MASTER

TECATE—A Code for Anisotropic Thermoelasticity in High-Average-Power Laser Technology

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INTRODUCTION

The attainment of high average power outputs from solid state lasers depends critically upon material properties of the laser host medium. For example, the relatively low thermal conductivities of Nd-doped glasses permit large thermal peaks to build up within the glass when flashlamp radiation is absorbed. These thermal peaks in turn generate large thermal stresses which can approach tensile yield strengths of laser glasses at rather modest average power levels. This type of thermal effect has been a major limiting factor in the attainment of high average power outputs from Nd: glass lasers.⁽¹⁾ Alternatively, various oxide and fluoride crystals are known to have thermal conductivities which exceed those of Nd: glass by an order of magnitude, or more. But anisotropic host media are subject to such optical propagation effects as stress-induced birefringence and biaxial focussing which may either degrade or completely halt effective laser operation. In addition to anisotropic thermal conductivities, other important anisotropic material properties include thermal expansion coefficients, elastic compliances and stiffness matrices, and stress-optic coefficients. The full composite of these and perhaps still other anisotropic physical effects in crystals must be understood quantitatively and also designed practically into future high average power laser systems which would use crystalline host media.

This report describes a totally Eulerian code for anisotropic thermo-elasticity (code name TECATE) which may be used in evaluations of prospective crystal media for high-average-power lasers. The present TECATE code version computes steady-state distributions of material temperatures, stresses, strains, and displacement fields in 2-D slab geometry. Numerous heat source and coolant boundary condition options are available in the TECATE code for laser design considerations. Anisotropic analogues of plane stress and plane strain evaluations can be executed for any and all crystal symmetry classes. As with all new and/or large physics codes, it is likely that some code imperfections will emerge at some point in time. It is also anticipated that some code users may encounter applications needs which are not addressed in this original TECATE code version. The authors will make every possible effort to service such user needs as they materialize and become known to us.

This report is organized as follows: Section I presents physics formulations for computing both the flow of heat and the induced thermal stresses, strains, and displacements in anisotropic media. Section II considers TECATE code solutions of anisotropic thermoelastic stress effects; this section discusses some code validation problems and some sample problems of crystals in practical thermal environments. Section III presents sample working sessions of the TECATE code, as it was used to set up and solve some of the problems which were discussed in Section II. Appendix 1 contains a preprint of a journal article which describes in extensive detail the mathematical formulations and numerical analysis features of the PDE solution methods in the TECATE code. Appendix 2 contains 3-D elastic compliance matrix structures for all crystal systems, and Appendix 3 contains thermoelastic material data for those crystal systems which are considered in this report.

I. PROBLEM FORMULATION

The TECATE code solves steady state heat and thermoelastic stress equations in 2-D slab geometry. In order to facilitate parametric studies of arbitrary crystal media in various physical environments, TECATE code users may elect to execute either pre-coded options which exist within the basic TECATE program or their own encoded formulations (via supplemental subroutines) of heat sources, coolant flows, slab configurations, and boundary conditions.

Figures 1a-1c represent three basic flow configurations which are presently computed in the TECATE code; these may be referred to subsequently as co-flow, counterflow and transverse flow configurations. It is assumed that heat sources within slab laser media are generated by the absorption of flashlamp radiation in the laser host medium. Heat source options within TECATE include: (i) precoded flashlamp absorption models for either one-sided or two-sided illumination, and (ii) subroutines which will accommodate user-encoded heat sources with nearly arbitrary functional forms in 2-D slab geometry. Computations of heat transfer from a slab laser material to an ambient coolant medium can currently use the following boundary condition options: (i) heat flux conditions with non-zero, finite film coefficients at the boundaries; (ii) adiabatic (zero-Neumann) boundary conditions; and (iii) arbitrary specifications of temperature values along slab boundaries. (Descriptions of these various source function and boundary condition options appear in subsequent sections.) Users may also elect to simply provide in a supplemental subroutine their own known temperature distribution; under this option the heat transfer portion of the TECATE code is by-passed altogether, and only the material stresses, strains, and displacements are computed.

A. HEAT FLOW IN ANISOTROPIC MEDIA

The generalized heat equation can be written as

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (\underline{k} \cdot \nabla T) + Q \quad (1)$$

Figure 1a. Co-Flow Configuration

Figure 1b. Counter-Flow Coolant Configuration

Figure 1c. Transverse Flow Configuration

where $T \equiv$ temperature (degrees)
 $\rho \equiv$ mass density (mass/volume)
 $c \equiv$ heat capacity (energy/mass-degree)
 $\underline{k} \equiv$ thermal conductivity tensor (power/length-degree)
 $\underline{Q} \equiv$ rate of internal heat generation (power/volume)

At steady-state, $\lim_{t \rightarrow \infty} \frac{\partial T}{\partial t} \rightarrow 0$, and Equation (1) can be written as

$$\nabla \cdot (\underline{k} \cdot \nabla T) = -Q \quad (2)$$

The elements of the thermal conductivity matrix, k_{ij} , have been treated as constants in this initial code version. This assumption can be relaxed, as necessary,⁽²⁾ to permit $\underline{k}$ to be a general function of x , y , and T .

Figure 2 indicates schematically the 2-D slab geometry which is used in TECATE code computations. The heat equation is solved using a nine-point, second-order accurate differencing scheme. Complete details of the numerical methods which are used in TECATE for solving both the heat and thermoelastic stress equations appear in Appendix 1. We briefly summarize here the numerical approach which is used for the solution of the heat equation.

Figure 2. Schematic Representation of 2-D Slab Geometry Which is Used For Heat and Stress in TECATE Code Computations of Anisotropic Solid Materials.

A first step in the numerical solution of the heat equation is a transformation of Equation (2) from laboratory co-ordinates (X,Y) onto the domain of the unit square, whose co-ordinates are denoted by (x,y) (see Figure 3). This transformation is given by the following relationships:

$$y = Y/HT \quad , \quad (3)$$

$$x = \frac{X - (\cot \alpha) \cdot Y}{WIDTH} \quad (4)$$

We note that, on the domain Ω (see Figure 3), T and Q are functions of X and Y , whereas on the unit square, T and Q become functions of x and y through the use of the inverse transformation given by (3) and (4). One may then write,

$$\begin{aligned} T &= T(X,Y) = T(X(x,y),Y(x,y)) \equiv T'(x,y) \quad , \\ Q &= Q(X,Y) = Q(X(x,y),Y(x,y)) \equiv Q'(x,y) \quad . \end{aligned} \quad (5)$$

Because we will be working mostly on the unit square, the primes in Equation (5) can be dropped henceforth for convenience. A similar convention will be used in the stress analysis sections.

Equation (2) can be written in the laboratory frame as

$$\nabla \cdot \underline{k} \cdot \nabla T = k_{11} T_{XX} + 2k_{12} T_{XY} + k_{22} T_{YY} = -Q \quad . \quad (6)$$

Applying the chain rule,

$$\frac{\partial}{\partial X} = \frac{\partial x}{\partial X} \frac{\partial}{\partial x} + \frac{\partial y}{\partial X} \frac{\partial}{\partial y} = \left(\frac{1}{WIDTH} \right) \cdot \frac{\partial}{\partial x} \quad (7)$$

$$\frac{\partial}{\partial Y} = \frac{\partial x}{\partial Y} \frac{\partial}{\partial x} + \frac{\partial y}{\partial Y} \frac{\partial}{\partial y} = \left(\frac{1}{HT} \right) \cdot \frac{\partial}{\partial y} - \left(\frac{\cot \alpha}{WIDTH} \right) \frac{\partial}{\partial x} \quad , \quad (8)$$

it follows that

Figure 3. Schematic Representation of the Transformation from Laboratory Co-ordinates (X,Y) onto the domain of the Unit Square (x,y) .

$$T_{XX} = \frac{1}{(\text{WIDTH})^2} T_{xx} \quad (9)$$

$$T_{XY} = \frac{1}{HT \cdot \text{WIDTH}} T_{xy} - \frac{\cot \alpha}{(\text{WIDTH})^2} T_{xx} \quad (10)$$

$$T_{YY} = \frac{1}{(HT)^2} T_{yy} - \frac{2 \cot \alpha}{HT \cdot \text{WIDTH}} T_{xy} + \left(\frac{\cot \alpha}{\text{WIDTH}} \right)^2 T_{xx} \quad (11)$$

Equation (2) can be written on the domain of the unit square as

$$\underline{\nabla} \cdot (\underline{K} \cdot \underline{\nabla} T) = -Q \quad , \quad (12)$$

where

$$\underline{K} = \begin{bmatrix} K_{11} & K_{12} \\ K_{12} & K_{22} \end{bmatrix} \quad , \quad (13)$$

and

$$K_{11} = \frac{1}{(WIDTH)^2} \{ k_{11} - 2\cot\alpha \cdot k_{12} + (\cot\alpha)^2 k_{22} \} \quad (14)$$

$$K_{12} = \frac{1}{HT \cdot WIDTH} \{ k_{12} - \cot\alpha \cdot k_{22} \} \quad (15)$$

$$K_{22} = \frac{1}{(HT)^2} k_{22} \quad (16)$$

1. Boundary Conditions

The following boundary conditions may hold in the laboratory frame:

(i) Dirichlet Condition

$$T = \text{some designated function } F \text{ on } \partial\Omega_1 \text{ (Dirichlet)} , \quad \text{and} \quad (17)$$

(ii) Flux (Neumann) Condition

$$(\underline{k} \cdot \underline{\nabla} T) \cdot \underline{\hat{m}} = h(T_c - T) \text{ on } \partial\Omega_2 \text{ (Neumann)} , \quad (18)$$

where the intersection of $\partial\Omega_1$ and $\partial\Omega_2$ is empty, and their union is the entire boundary of the slab cross section $\partial\Omega$. To insure uniqueness of the solution when $h = 0$, $\partial\Omega_1$ must contain at least one point. The unit outer normal to the boundary surface is denoted by $\underline{\hat{m}}$; T_c is the ambient coolant temperature; and h is a positive coefficient for heat transfer across the boundary (power/(length)² - degree). Referring to Figure 4, it can be seen that the Neumann boundary conditions on the boundary of the unit square $\partial\Omega$ are given by:

$$(\underline{k} \cdot \underline{\nabla} T) \cdot \underline{\hat{n}} = \frac{h}{WIDTH \cdot \sin\alpha} \cdot (T_c - T) \text{ on } \textcircled{2} \text{ and } \textcircled{4} , \quad (19)$$

$$\text{and } (\underline{k} \cdot \underline{\nabla} T) \cdot \underline{\hat{n}} = \frac{h}{HT} \cdot (T_c - T) \text{ on } \textcircled{1} \text{ and } \textcircled{3} . \quad (20)$$

Figure 4. Schematic Representation of Boundary Condition Transformation from the Laboratory Frame to the Unit Square.

Numerical solution of the transformed heat equation (as well as the transformed stress potential equation) on the unit square offers several potential advantages including: (i) differential operators are more easily differenced in the (x,y) frame than in the laboratory frame; (ii) extensive error-analysis can be performed in the (x,y) frame, which permits highly effective differencing schemes to be implemented--both at the interior and at the slab boundaries; and (iii) ADI methods which are used to solve the steady state heat and stress potential equations in 2-D are better posed in the (x,y) frame than in the laboratory frame.⁽³⁾ The full impact of these numerical properties becomes apparent as increasingly difficult practical problems are undertaken, as discussed in later sections.

2. Flashlamp Source Functions

A standard heat source model in the TECATE code is derived from the flashlamp absorption efficiency model which has been used previously for Nd-doped glass lasers.⁽⁴⁾ Recall that the efficiency ϵ of storing extractable laser energy in a volume with "thickness" l is measured and fitted to the function

$$\epsilon(l) = A[1 - B \exp(-C\rho_n l) - (1 - B) \exp(-D\rho_n l)] \quad , \quad (21)$$

where $\rho_n \equiv \text{Nd}^{3+}$ (dopant) density .

The coefficients (A, B, C, D) can be tabulated in data arrays for various flashlamp parameters and various laser media. The source rate of storing extractable energy in an infinitesimal thickness dY about Y from a flashlamp source at $Y = 0$ is given by

$$Q_0(Y) \equiv \frac{\partial \epsilon}{\partial l} \bigg|_{l=Y-0} = A[BC\rho_n \exp(-C\rho_n Y) + (1-B) D\rho_n \exp(-D\rho_n Y)] \quad (22)$$

Similarly, for a source of illumination at $Y = HT$,

$$Q_{HT}(Y) \equiv \frac{\partial \epsilon}{\partial l} \bigg|_{l=HT-Y} = A[BC\rho_n \exp(-C\rho_n (HT-Y)) + (1-B) D\rho_n \exp(-D\rho_n (HT-Y))] \quad (23)$$

We now wish to use these flashlamp source rate functions to represent the deposition of thermal energy in the laser medium rather than the deposition of extractable laser energy in the medium. We note that

$$\lim_{l \rightarrow \infty} \epsilon(l) = A \quad , \quad (24)$$

which states that, for a practically infinite slab, the efficiency ϵ is simply the fraction of extractable laser energy which is stored in the slab relative to the total flashlamp energy input to the slab. A two-sided heat source function Q can be obtained by a simple renormalization of the deposition functions Q_0 and Q_{HT} above. That is, one can define for the local deposition of heat in a slab which is illuminated by a flashlamp along its bottom boundary surface (at $Y=0$)

$$Q \begin{matrix} (Y) \\ \text{BOTTOM} \end{matrix} = \text{BOTPWR}[BC\rho_n \exp(-C\rho_n Y) + (1-B) D\rho_n \exp(-D\rho_n Y)] \quad . \quad (25)$$

Similarly, for illumination by flashlamps which are located along the top slab surface (at $Y = HT$), one can define the local heat deposition function

$$Q(Y) = \text{TOPPWR} \left[B C \rho_n \exp(-C \rho_n (HT - Y)) + (1 - B) D \rho_n \exp(-D \rho_n (HT - Y)) \right] , \quad (26)$$

and, finally,

$$Q = Q_{\text{BOTTOM}} + Q_{\text{TOP}} . \quad (27)$$

It can be shown that, for unit area,

$$\int_0^{HT} Q \, dy = (\text{TOPPWR} + \text{BOTPWR}) [1 - B \exp(-C \rho_n HT) - (1 - B) \exp(-D \rho_n HT)] , \quad (28)$$

and that

$$\lim_{HT \rightarrow \infty} \int_0^{HT} Q \, dy \rightarrow \text{TOPPWR} + \text{BOTPWR} , \quad (29)$$

where TOPPWR and BOTPWR are the total power levels per unit area which can be absorbed as heat in a laser slab due to illumination by flashlamps along the top and bottom slab surfaces, respectively. Alternative flashlamp heating models can also be implemented readily in the TECATE code.

3. Crystal Physics Conventions Used in TECATE Code Formulations

Neumann's Principle is one of the fundamental postulates of crystal physics. This principle states that each physical constant must include every element of symmetry in the point group of the crystal under consideration.* For example, if a crystal has three principal conductivity elements

*It does not follow from Neumann's principle that the symmetry elements of a physical property are entirely the same as those of the point group of a crystal. For example, the physical properties may possess more symmetry than the point group.

(i.e., expressed in the irreducible representation of the principal axes), each one of the conductivities must satisfy the symmetry of the crystal. Similarly, Neumann's Principle requires compliance of such physical properties as thermal expansion, elasticity, stress-optical, and piezo-electric effects, etc., with the symmetry of the crystal. The symmetry conventions adopted in TECATE code formulation follow closely the prescriptions of Nye,⁽⁵⁾ who has in turn followed closely the notation and terminology found in the International Tables for X-Ray Crystallography⁽⁶⁾ and the IRE Standards on Piezoelectric Crystals.⁽⁷⁾ The major features of those crystal conventions and principles which are used in TECATE code formulations are summarized immediately below.

It is useful to think of atoms occurring in crystals as small groups, with all groups exactly alike and similarly oriented in regular alignments in all dimensions. Each such grouping of atoms can be visualized as being bounded by a parallelepiped. The parallelepipeds are referred to as unit cells and serve as the basic building blocks of matter. Physical properties of crystals are described in terms of that natural co-ordinate system which is formed by axes which are parallel to the edges of a unit cell (see Figure 5). Arbitrary relationships between the axes U_a , U_b , U_c (or simply a , b , c)

Figure 5. Crystal axes are shown by the sides of a unit cell, U_a , U_b , U_c , where a_0 , b_0 , and c_0 are the lengths of the unit cell. Interaxial angles are denoted by α , β , γ .

and the right-handed rectangular frame x_1, x_2, x_3 , underlie many of the conventions which are used in crystal physics. In these conventions x_3 is taken along c , and x_2 is taken to be normal to the ac plane. The following rules define the positive a, b, c and x_1, x_2, x_3 axes:

- (i) $+x_3$ is parallel to $+c$ (and is hence parallel to the (100) and (010) planes).
- (ii) $+x_1$ is perpendicular to c in the ac plane, pointing in the general direction of $+a$. (x_1 is thus parallel to the (010) plane.)
- (iii) $+x_2$ is normal to the ac plane (010), pointing in the general direction of $+b$.

Table 1 summarizes the conventions for assignments of orthogonal axes (x_1, x_2, x_3) relative to the crystallographic axes in the seven basic crystal systems. With these assignments, the tensor structure for such quantities as thermal conductivities (second-rank tensors), elastic constants (fourth-rank tensors), etc., can then be designated. These designations of tensor elements are given below in terms of the crystal co-ordinate conventions indicated in Table 1. Thermal conductivities are given for the seven crystal systems as follows:

Triclinic system. There is no simplification, and

$$\underline{k} = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{pmatrix} . \quad (30)$$

If the x_3 -component is neglected in 2-D calculations,

$$\underline{k} = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix} . \quad (31)$$

Table 1
CRYSTAL SYSTEM CONVENTIONS

Crystal System	Convention for Assignment of a, b, c axes	Orientation of x_1, x_2, x_3 axes			Optical Classification
		x_1	x_2	x_3	
Triclinic	$c_0 < a_0 < b_0; \alpha, \beta > 90^\circ$		$\perp (010)$	c	Biaxial
Monoclinic*	$c_0 < a_0; \beta > 90^\circ; \alpha = \gamma = 90^\circ$	$\perp (100)$	b	c	Biaxial
Orthorhombic	$c_0 < a_0 < b_0; \alpha = \beta = \gamma = 90^\circ$	a	b	c	Biaxial
Isometric (Cubic)	$a_0 = b_0 = c_0; \alpha = \beta = \gamma = 90^\circ$	a	b	c	Isotropic (anaxial)
Tetragonal	$a_0 = b_0; \alpha = \beta = \gamma = 90^\circ$	a		c	Uniaxial
Trigonal	a and b are equivalent axes with unit cell lengths of a_0	a		c	Uniaxial
Hexagonal	a and b are equivalent axes with unit cell lengths of a_0	a		c	Uniaxial

*b is taken to be the unique crystal axis; this axis is most frequently oriented parallel to x_2 , in accordance with Reference 7.

Monoclinic system. If the x_3 -axis is either the diad axis or a normal to the plane of reflection symmetry

$$\underline{k} = \begin{pmatrix} k_{11} & k_{12} & 0 \\ k_{21} & k_{22} & 0 \\ 0 & 0 & k_{33} \end{pmatrix} . \quad (32)$$

Although it doesn't follow from symmetry arguments, which are frequently valid in elasticity theory, k_{21} is generally equal to k_{12} . If the x_2 -axis⁽⁷⁾ is taken to be the diad axis, the conductivity tensor is given in short hand notation by

$$\underline{k} = \begin{pmatrix} \bullet & - & \bullet \\ & \bullet & - \\ & & \bullet \end{pmatrix} . \quad (33)$$

where the dashes denote zeroes, and the solid dots denote non-zero matrix element values. Matrix symmetry is denoted in this convention by displaying conductivity matrix elements for only the upper diagonal matrix element locations.

Orthorhombic system.

$$\underline{k} = \begin{pmatrix} \bullet & - & - \\ & \bullet & - \\ & & \bullet \end{pmatrix} \quad (34)$$

Isotropic system.

$$\underline{k} = \begin{pmatrix} \bullet & - & - \\ & \bullet & - \\ & & \bullet \end{pmatrix} , \quad (35)$$

where the connecting lines between solid dots designate equal components, i.e., $k_{11} = k_{22} = k_{33}$.

Tetragonal, Trigonal, and Hexagonal systems.

$$\underline{k} = \begin{pmatrix} \bullet & - & - \\ & \bullet & - \\ & & \bullet \end{pmatrix} , \quad (36)$$

where the principal conductivities are related as $k_{22} = k_{11} \neq k_{33}$.

In many practical cases, the configuration of a cut crystal will suggest an optimal orientation of laboratory coordinates for computations which coincides with neither the natural axes of the unit cell nor the conventional orthogonal axes (x_1, x_2, x_3) discussed above. In such cases, TECATE code users must transform the thermal conductivity and other tensor elements from the conventional (x_1, x_2, x_3) frame indicated in Table 1 onto the particular laboratory frame of their specific applications. TECATE code input data must be provided to the code in that particular laboratory frame. The transformation conventions which are tacitly used in the modeling of crystal physics problems can be described in terms of Nye's notation⁽⁵⁾, as depicted both in Figure 6 and in the equations which appear in the discussion below. We assume for purposes of illustration that a crystal cross-section in the X-Y plane of the laboratory frame is a parallelogram (as shown in Figure 6) and that Z is not permitted to be a PDE independent variable in these 2-D computations. The "base" surface of the cut crystal is taken to include the X-axis. In this case, the orthogonal axes x_1 , x_2 and x_3 which are associated with the crystal symmetry conventions may have the direction cosines denoted by a_{ij} for $i, j = 1, 2, 3$ relative to the laboratory

Figure 6. Transformation of Axes in the x - y Plane.

co-ordinate frame (X,Y,Z). The first index of the a's refers to the "new" axes, and the second index refers to the "old" axes (see Figure 6).

It is convenient to tabulate the direction cosines of the "new" axes with respect to the "old" axes as

	x^{Old}	y^{Old}	z^{Old}
x^{New}	a_{11}	a_{12}	a_{13}
y^{New}	a_{21}	a_{22}	a_{23}
z^{New}	a_{31}	a_{32}	a_{33}

A vector $\underline{p}$ thus transforms as

$$p_i^{New} = a_{ij} p_j^{Old} \quad i, j = 1, 2, 3 \quad (37)$$

and

$$p_i^{Old} = a_{ji} p_j^{New} \quad i, j = 1, 2, 3 \quad (38)$$

(We note in Equation (37) that, for the "new" quantity expressed in terms of the "old", the repeated (dummy) indices occur in neighboring locations; whereas the repeated indices are separated in the reverse transformation.)

Whereas Equations (37) and (38) indicate that first-rank tensors (vectors) transform the same as co-ordinate points, one finds that such second-rank tensors as thermal conductivities transform the same as products of co-ordinates. That is,

$$k_{ij}^{New} = a_{ik} a_{jl} k_{kl}^{Old} \quad i, j, k, l = 1, 2, 3 \quad (39)$$

or in the $x_1 - x_2$ plane (ignoring x_3 and z)

$$k_{ij}^{New} = a_{i1} a_{j1} k_{11}^{Old} + a_{i1} a_{j2} k_{12}^{Old} + a_{i2} a_{j1} k_{21}^{Old} + a_{i2} a_{j2} k_{22}^{Old} \quad (40)$$

Similarly,

$$k_{ij}^{Old} = a_{ki} a_{lj} k_{kl}^{New} \quad i, j, k, l = 1, 2, 3 \quad (41)$$

Thermoelasticity formulations and computations involve fourth-rank tensors; the conventions for these higher-rank tensors will be discussed in the next section.

B. THERMOELASTICITY IN ANISOTROPIC MEDIA

In order to formulate the thermoelastic equations efficiently, we again follow the conventions of Nye.⁽⁵⁾ The strain ϵ_{ij} is defined as

$$\epsilon_{ij} \equiv \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) = \epsilon_{ji} \quad i, j = 1, 2, 3, \quad (42)$$

where u_i denotes a component of the displacement u in the direction of coordinate x_i . The strain ϵ_{ij} is a second-rank tensor and can be viewed as the symmetric part of the displacement variation (or deformation) $e_{ij} = \frac{\partial u_j}{\partial x_i}$. The antisymmetric tensor ω_{ij} is referred to as the rotation and is defined as $\omega_{ij} \equiv \frac{1}{2} (e_{ij} - e_{ji})$.

A general deformation is expressed by the relationship,

$$e_{ij} = \epsilon_{ij} + \omega_{ij} \quad (43)$$

NOTE: Readers of this report and users of the TECATE code are cautioned that a single standard convention for strain definitions does not exist. For example, such notable authors as Lekhnitskii⁽⁸⁾ define ϵ_{ij} to be equal to $(e_{ij} + e_{ji})$ rather than $\frac{1}{2}(e_{ij} + e_{ji})$. We therefore adhere strictly to the conventions defined by Equations (42)-(43) in all TECATE code work.

If the temperature of a crystal undergoes variation δT , the components of ϵ_{ij} are proportional to δT as

$$\epsilon_{ij} \sim \alpha_{ij} \delta T, \quad (44)$$

where α_{ij} are coefficients of thermal expansion which are assumed to be constant in current TECATE code versions.

Hooke's law, expressed in general form, is

$$\epsilon_{ij} = s_{ijkl} \sigma_{kl} + \alpha_{ij} \delta T, \quad i, j, k, l = 1, 2, 3, \quad (45)$$

where the stress tensor (cf second-rank) is denoted by the elements σ_{kl} , and the compliances s_{ijkl} are elements of a fourth-rank tensor.

An alternative representation of Hooke's law is

$$\sigma_{ij} = c_{ijkl} (\epsilon_{kl} - \alpha_{kl} \delta T), \quad (46)$$

where c_{ijkl} denotes the stiffnesses, or elastic constants, of a material.

The compliances transform as

$$s_{ijkl}^{\text{New}} = a_{im} a_{jn} a_{ko} a_{lp} s_{mnop}^{\text{Old}}, \quad (47)$$

and it can be shown that

$$s_{ijkl} = s_{jikl} = s_{ijlk} \quad (48a)$$

$$s_{ijkl} = s_{klij} \quad (48b)$$

$$c_{ijkl} = c_{jikl} = c_{ijlk} \quad (48c)$$

$$c_{ijkl} = c_{klij} \quad (48d)$$

The symmetry expressed above for the first two and the last two indices of s and c permit the use of a very effective matrix notation, which is now in widespread use. In this notation, pairs of tensor indices are abbreviated into a single matrix index as follows:

tensor notation:	11	22	33	23,32	31,13	12,21
matrix notation:	1	2	3	4	5	6

Stresses and strains are then denoted by

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \rightarrow \begin{pmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{pmatrix} \quad (49)$$

$$\begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{pmatrix} \rightarrow \begin{pmatrix} \epsilon_1 & \frac{1}{2}\epsilon_6 & \frac{1}{2}\epsilon_5 \\ \frac{1}{2}\epsilon_6 & \epsilon_2 & \frac{1}{2}\epsilon_4 \\ \frac{1}{2}\epsilon_5 & \frac{1}{2}\epsilon_4 & \epsilon_3 \end{pmatrix} \quad (50)$$

The factors of $\frac{1}{2}$ appear in Equation (50) as a result of the convention selected in Equations (42)-(44). This convention maintains certain symmetry and spatial transformation properties; and it has the practical effect of eliminating factors of 2 and 4 in ensuing summations which occur in the compact notation for s_{ijkl} by requiring that the following relationships hold between the full tensor notation and the compact notation,

$$s_{ijkl} = s_{mn}, \text{ and } \alpha_{ij} = \alpha_m \quad m, n = 1, 2, 3 \quad (51a)$$

$$2s_{ijkl} = s_{mn} \quad \text{either } m \text{ or } n = 4, 5, 6 \quad (51b)$$

$$4s_{ijkl} = s_{mn} \quad \text{both } m, n = 4, 5, 6, \quad (51c)$$

$$2\alpha_{ij} = \alpha_m \quad m = 4, 5, 6 \quad (51d)$$

Hooke's law is written in compact notation as

$$\epsilon_m = s_{mn} \sigma_n + \alpha_m \delta T \quad m, n = 1, 2, \dots, 6 \quad (52)$$

Similarly,

$$\sigma_m = c_{mn} \epsilon_n - c_{mn} \alpha_n \delta T \quad m, n = 1, 2, \dots, 6 \quad (53)$$

where (noting the absence of factors of 2 and/or 4)

$$c_{ijkl} = c_{mn} \quad i, j, k, l = 1, 2, 3; m, n = 1, \dots, 6 \quad (54)$$

It is well for the reader to become familiar with these conventions (which may initially seem confusing) by writing out some of the basic expressions. For example, the full tensor form of Equations (42) and (45) gives

$$\begin{aligned} \epsilon_{11} = & s_{1111} \sigma_{11} + s_{1112} \sigma_{12} + s_{1113} \sigma_{13} + s_{1121} \sigma_{21} + s_{1122} \sigma_{22} + s_{1123} \sigma_{23} \\ & + s_{1131} \sigma_{31} + s_{1132} \sigma_{32} + s_{1133} \sigma_{33} + \alpha_{11} \delta T \quad (55) \end{aligned}$$

Using Equations (50)-(51) in conjunction with the symmetry properties of the compliances, Equation (55) can be written in compact notation as

$$\begin{aligned} \epsilon_1 = & s_{11} \sigma_1 + \frac{1}{2} s_{16} \sigma_6 + \frac{1}{2} s_{15} \sigma_5 + \frac{1}{2} s_{16} \sigma_6 + s_{12} \sigma_2 + \frac{1}{2} s_{14} \sigma_4 + \frac{1}{2} s_{15} \sigma_5 + \\ & \frac{1}{2} s_{14} \sigma_4 + s_{13} \sigma_3 + \alpha_1 \delta T \quad (56) \end{aligned}$$

By gathering terms, one obtains

$$\epsilon_1 = s_{1n} \sigma_n + \alpha_1 \delta T \quad n = 1, \dots, 6 \quad (57a)$$

and in general

$$\epsilon_m = s_{mn} \sigma_n + \alpha_m \delta T \quad m = 1, 2, 3; n = 1, \dots, 6 \quad (57b)$$

Similarly, the compact expression for $\epsilon_{21} = \epsilon_{12}$ is given by

$$\frac{1}{2}\epsilon_6 = \frac{1}{2}s_{61}\sigma_1 + \frac{1}{4}s_{66}\sigma_6 + \frac{1}{4}s_{65}\sigma_5 + \frac{1}{4}s_{66}\sigma_6 + \frac{1}{2}s_{62}\sigma_2 + \frac{1}{4}s_{64}\sigma_4 + \frac{1}{4}s_{65}\sigma_5 + \frac{1}{4}s_{64}\sigma_4 + \frac{1}{2}s_{63}\sigma_3 + \frac{1}{2}\alpha_6\delta T, \quad (58)$$

which simply becomes

$$\epsilon_6 = s_{6n}\sigma_n + \alpha_6\delta T, \quad n = 1, \dots, 6, \quad (59a)$$

and in general

$$\epsilon_m = s_{mn}\sigma_n + \alpha_m\delta T, \quad m = 4, 5, 6; n = 1, \dots, 6. \quad (59b)$$

It is important to note that the compact matrices s_{mn} and c_{mn} do not transform as tensors. The compact matrices should be converted back to s_{ijkl} when spatial co-ordinate transformations are to be performed; the fourth-rank compliance and stiffness tensors s_{ijkl} and c_{ijkl} are then transformed according to Equation (47). Preprocessing routines which perform arbitrary rotation transformations on s_{ijkl} and c_{ijkl} in 3-D are available from the authors of this report for use in conjunction with the TECATE program.

1. Reduction to 2-D Thermoelastic Formulations

The standard reductions of 3-D thermoelastic equations to 2-D scalar stress potential equations for isotropic "plane stress" and "plane strain" problems^(9,10) require some modifications when similar reductions are undertaken for anisotropic media. Referring to Figure 7, we can recall the conditions of isotropic "plane strain" in a prismatic body of infinite length with no body forces. That is, the displacement component u_3 in the axial direction Z is zero, and the remaining two displacement components u_1 and u_2 are functions of only X and Y .⁽⁹⁾ With the use of these conditions as a semi-inverse assumption, it can be shown that "plane strain" is realized in isotropic media when the following relationships hold:

$$\epsilon_{13} = \epsilon_{23} = \epsilon_{33} = 0 \quad (60)$$

$$\epsilon_{11} = \epsilon_{11}(X, Y); \epsilon_{22} = \epsilon_{22}(X, Y); \epsilon_{12} = \epsilon_{12}(X, Y) \quad (61)$$

$$\sigma_{13} = \sigma_{23} = 0 \quad (62)$$

The stress component σ_{33} is evaluated from the constitutive equation for ϵ_{33} and is found to be

$$\sigma_{33} = \nu(\sigma_{11} + \sigma_{22}) - \alpha^T E \delta T, \quad (63)$$

where ν is Poisson's ratio; E is Young's modulus, and α^T is a scalar thermal expansion co-efficient. It also follows that the temperature variation δT is a function of only X and Y and that the boundary tractions must also be independent of Z . Under these conditions, an isotropic body would experience plane deformation in which all cross sections of the solid material normal to the Z -axis in Figure 7 would remain planar, and the stresses and displacements would depend only upon X and Y .*

Figure 7. Prism of Solid Material of Infinite Length for Discussion of Reductions of 3-D Thermoelastic Equations to 2-D in Both Isotropic and Anisotropic Media. Laboratory Co-ordinates are Represented by the Orthogonal X , Y , Z Axes. At Equilibrium $\nabla \cdot \underline{\underline{\sigma}} = \underline{\underline{F}}$.

*It is assumed that rotations about the X and Y axes without deformation are excluded.

2. Generalized Plane Deformation in Anisotropic Media

In a general anisotropic body, some of the plane deformation features mentioned above for isotropic media are not fully attainable because it is impossible to satisfy the equilibrium equations

$$\nabla \cdot \underline{\underline{\sigma}} = \underline{\underline{F}} \quad (64)$$

for the condition of $u_3 = 0$. In order to satisfy the equilibrium conditions for generalized plane deformations in anisotropic media, the defining relationships must be relaxed so that: (i) all components of stresses and displacements are independent of Z , and (ii) temperature variations δT and boundary conditions are also independent of Z . From these conditions, two cases of generalized plane deformation can be realized in 2-D models of anisotropic bodies:

(i) In the first instance of pure planar deformation, axial displacements u_3 are simply constant; and initially planar cross sections normal to the Z -axis remain planar. It follows from Equation (42) that $\epsilon_3 = 0$. In those anisotropic cases in which $s_{14} = s_{24} = s_{34} = s_{64} = s_{15} = s_{25} = s_{35} = s_{65} = 0$,

$$\sigma_3 = -\frac{1}{s_{33}} (s_{13}\sigma_1 + s_{23}\sigma_2 + s_{36}\sigma_6 + \alpha_3\delta T) , \quad (65)$$

in strict analogy to the case of "plane strain" in isotropic media. Whereas this set of specialized conditions on compliances and elastic stiffnesses may hold in the conventional frame $\{x_1, x_2, x_3\}$ for orthorhombic, cubic, tetragonal, and hexagonal crystals; non-zero compliances for s_{m4} and s_{m5} , $m = 1, 2, 3, 6$, may be present when such crystals are cut in certain other orientations. Users of this version of TECATE, which computes only purely planar deformations, must therefore be especially mindful of the structure of compliance matrices in arbitrary crystal orientations.

(ii) In the second instance, arbitrary compliance elements s_{m4} and s_{m5} can be considered theoretically in 2-D for all m by the introduction

of a second stress potential function $\psi(X,Y)$ and one additional compatibility equation. The equilibrium conditions which were indicated above apply also in this instance. It is again required that axial displacements u_3 be functions of only X and Y and that temperature loadings must remain independent of Z . It then follows that $\sigma_1, \sigma_2, \sigma_4, \sigma_5, \sigma_6$ can be computed explicitly from the two potentials ϕ and ψ and that σ_3 is computed algebraically from Equation (52) using the fact that $\epsilon_3 = 0$. This type of computation will sometimes be referred to as a "2 1/2-D" model. In presently unreported work, the TECATE code has been temporarily modified and tested for such generalized planar deformations; and some interesting preliminary results have been obtained for nonplanar axial displacements in trigonal crystals in their conventional frame. A generalized 2 1/2-D TECATE code version, including physical examples, will be reported separately in a future document. (In the meantime interested readers may wish to peruse both Appendix 1 and Reference 10.) Notwithstanding the numerous modifications of the isotropic "plane strain" concept which must be invoked in considerations of anisotropic media, the case of plane deformation in practically infinite slabs remains the most physically useful option of the TECATE code in computations of anisotropic crystals.

3. Plane Deformation in Finite Slabs of Anisotropic Media

The analog of isotropic "plane stress" is introduced by considering a thin anisotropic material slab which is normal to the Z -axis in Figure 3. That is, we consider two planes normal to the Z -axis which are separated by a finite thickness h which is small relative to the cross-section dimensions. The semi-inverse assumption of 2-D isotropic "plane stress" in which the slab faces are free of forces and the mid-plane of the slab remains planar while undergoing deformation is

$$\sigma_3 = \sigma_4 = \sigma_5 = 0 \quad (66)$$

It is found that such a state of stress can exist within the context of the 3-D thermoelastic theory only in specialized circumstances which require the

Figure 8. Thin Material Slab Considered in Isotropic "Plane Stress" and in Anisotropic Plane Deformation.

temperature distribution to satisfy $\nabla^2 \delta T = f(Z)$ and/or equilibrating boundary forces to be defined on the slab edges.⁽⁹⁾ As indicated above, we are not presently considering laser applications which impose tractions on crystal edges. The development of 2-D stress potential equations for this case therefore appears in the TECATE code primarily in deference to its classic significance in isotropic studies.

4. Development of 2-D Stress Potential Equations for Anisotropic Media

Two-dimensional thermoelasticity problems with small displacements can be formulated in two representations: (i) a system of partial differential

equations for displacement components u_i can be developed and solved for problems which have clamped boundaries, and (ii) a scalar fourth-order stress potential equation can be developed and solved with high levels of accuracy and efficiency for problems with purely planar deformations and free boundaries. (Both approaches, however, can be extended, though not as efficiently, so as to include free boundary conditions in the first approach and clamped boundary conditions in the second approach.) For the second case, Airy's stress potential function, $\phi(X,Y)$, is introduced according to the definitions

$$\sigma_1 = \sigma_{XX} \equiv \frac{\partial^2 \phi}{\partial Y^2} \quad ; \quad (67a)$$

$$\sigma_6 = \sigma_{XY} \equiv -\frac{\partial^2 \phi}{\partial X \partial Y} \quad ; \quad (67b)$$

$$\sigma_2 = \sigma_{YY} \equiv \frac{\partial^2 \phi}{\partial X^2} \quad . \quad (67c)$$

In order to maintain compatibility of the overdetermined set of strain components and displacements, the following compatibility equation must be satisfied:

$$\frac{\partial^2 \epsilon_{XX}}{\partial Y^2} + \frac{\partial^2 \epsilon_{YY}}{\partial X^2} - 2 \frac{\partial^2 \epsilon_{XY}}{\partial X \partial Y} = 0 \quad , \quad (68)$$

or

$$\frac{\partial^2 \epsilon_1}{\partial Y^2} + \frac{\partial^2 \epsilon_2}{\partial X^2} - \frac{\partial^2 \epsilon_6}{\partial X \partial Y} = 0 \quad . \quad (69)$$

a. Analog of Isotropic "Plane Stress" in Finite Slabs

For ease of presentation, the anisotropic analog of isotropic "plane stress" is considered first. It is assumed that $\sigma_3 = \sigma_4 = \sigma_5 = 0$.

Equations (59b) of Hooke's Law are then differentiated appropriately for $m = 1, 2, 6$ so as to evaluate Equation (69) by direct substitution. The following scalar stress potential equation is obtained:*

$$s_{11}\phi_{YYYY} - (s_{16} + s_{61})\phi_{XYYY} - (s_{26} + s_{62})\phi_{XXXY} + (s_{12} + s_{21} + s_{66})\phi_{XXYY} \\ + s_{22}\phi_{XXXX} = -\alpha_1(\delta T)_{YY} - \alpha_2(\delta T)_{XX} + \alpha_6(\delta T)_{XY} \quad (70)$$

This is the stress potential equation which is solved in the TECATE code under what can be termed the "finite slab" or "plane stress" option for arbitrary crystal systems. The compliances and thermal expansion coefficients must be provided as input to the TECATE code in the laboratory co-ordinate frame of the calculation. For the familiar case of isotropic media, it is readily verified that Equation (70) reduces to the bi-harmonic equation,

$$\nabla^2 \nabla^2 \phi = \phi_{XXXX} + 2\phi_{XXYY} + \phi_{YYYY} = -E\alpha \nabla^2(\delta T) \quad (71)$$

where the following relationships hold:

$$E = 2G(1 + \nu) \quad (72)$$

$$s_{11} = s_{22} = s_{33} = \frac{1}{E} \quad (73)$$

$$s_{21} = s_{12} = s_{13} = s_{31} = s_{32} = s_{23} = -\frac{\nu}{E} \quad (74)$$

$$s_{66} = 2(s_{11} - s_{12}) = \frac{1}{G} \quad (75)$$

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha^T \quad (76)$$

with the shear modulus denoted by G .

*The symmetry properties $s_{mn} = s_{nm}$ have not yet been invoked in this derivation in order to indicate clearly the origin of the individual terms in Equation (70).

b. Analog of "Plane Strain" for Specific Crystal Symmetry Properties

It is assumed for the case of plane deformation that a prismatic slab of arbitrary crystalline material has essentially infinite length in the axial direction, which is taken to be the Z-axis in the laboratory frame. It is assumed that temperature variations δT are independent of Z and that boundary conditions are independent of Z. Under these conditions, the displacements u_1 , u_2 , and u_3 are independent of Z. It is assumed further that both surface tractions and body forces are zero. For these conditions, we wish to develop and solve a scalar stress potential equation as a function of X and Y in order to obtain values for σ_1 , σ_2 , and σ_6 according to Equations (67).

The condition $u_3 = u_3(X,Y)$ gives $\epsilon_3 = \partial u_3 / \partial z = 0$. It follows that σ_3 can be evaluated from Equation (59b) as

$$\sigma_3 = -\frac{1}{s_{33}} \left\{ \alpha_3 \delta T + s_{31} \sigma_1 + s_{32} \sigma_2 + s_{34} \sigma_4 + s_{35} \sigma_5 + s_{36} \sigma_6 \right\} \quad (77)$$

Because the stresses σ_4 and σ_5 are not accessible in this single potential theory, the compliances s_{34} and s_{35} in Equation (77) must be taken to be zero. We reiterate that this condition imposes a necessary restriction upon the crystal symmetry classes and crystal orientations (transformed compliances) which can be considered in the present single potential code. The compatibility Equation (69) implies further crystal symmetry restrictions, in that the strains ϵ_1 , ϵ_2 , and ϵ_6 must also be independent of σ_4 and σ_5 . It thus follows from Equation (59b), letting $m = 1, 2$, that we restrict current applications of TECATE to those crystal classes and orientations in which $s_{14} = s_{15} = s_{24} = s_{25} = s_{64} = s_{65} = 0$, in addition to $s_{34} = s_{35} = 0$ in the laboratory frame X, Y, Z. (This restriction will not be required in the generalized plane strain theory which incorporates an additional stress potential.) We note further that the above restrictions on the compliances do not imply that the quantities σ_4 and σ_5 are zero -- even for purely planar deformations. (Interested investigators can perform extended analyses on the 3-D compatibility and/or equilibrium equations to gain further insights into these conditions as viewed in terms of displacements or in terms of two stress potentials. See Appendix 1, also.)

The structural forms of the compliance and stiffness matrices in the conventional orthogonal axes (x_1, x_2, x_3) of Table 1 are shown in Appendix 2, and the scalar stress potential equation for purely planar deformation can now be developed as follows:

Equation (77) reduces to

$$\sigma_3 = -\frac{1}{s_{33}} \left\{ \alpha_3 \delta T + s_{31} \sigma_1 + s_{32} \sigma_2 + s_{36} \sigma_6 \right\}, \quad (78)$$

and substitution of Equation (78) into Equation (56) gives the expression

$$\epsilon_1 = s'_{11} \sigma_1 + s'_{12} \sigma_2 + s'_{16} \sigma_6 + \alpha'_1 \delta T, \quad (79)$$

where

$$s'_{11} \equiv s_{11} - \frac{s_{13}s_{31}}{s_{33}}, \quad (80)$$

$$s'_{12} \equiv s_{12} - \frac{s_{13}s_{32}}{s_{33}}, \quad (81)$$

$$s'_{16} \equiv s_{16} - \frac{s_{13}s_{36}}{s_{33}}, \quad (82)$$

$$\alpha'_1 \equiv \alpha_1 - \frac{s_{13}\alpha_3}{s_{33}}. \quad (83)$$

Similarly,

$$\epsilon_2 = s'_{2j} \sigma_j + \alpha'_2 \delta T \quad j = 1, 2, 6 \quad (84)$$

and

$$\epsilon_6 = s_{6j}' \sigma_j + \alpha_6' \Delta T, \quad j = 1, 2, 6, \quad (85)$$

where

$$s_{21}' \equiv s_{21} - \frac{s_{23}s_{31}}{s_{33}}, \quad (86)$$

$$s_{22}' \equiv s_{22} - \frac{s_{23}s_{32}}{s_{33}}, \quad (87)$$

$$s_{26}' \equiv s_{26} - \frac{s_{23}s_{36}}{s_{33}}, \quad (88)$$

$$\alpha_2' \equiv \alpha_2 - \frac{s_{23}\alpha_3}{s_{33}}, \quad (89)$$

$$s_{61}' \equiv s_{61} - \frac{s_{63}s_{31}}{s_{33}}, \quad (90)$$

$$s_{62}' \equiv s_{62} - \frac{s_{63}s_{32}}{s_{33}}, \quad (91)$$

$$s_{66}' \equiv s_{66} - \frac{s_{63}s_{36}}{s_{33}}, \quad (92)$$

$$\alpha_6' \equiv \alpha_6 - \frac{s_{63}\alpha_3}{s_{33}}. \quad (93)$$

It can readily be shown that the potential equation for the purely planar deformation is structurally identical to Equation (70). All of the terms s_{mn} and α_m in Equation (70) are simply replaced by the corresponding terms s_{mn}' and α_m' defined in Equations (80)-(93) in order to

obtain the scalar potential equation for purely planar deformation in anisotropic media. (We will henceforth not use a separate stress potential equation with primed coefficients to apply to the case of purely planar deformation; it is understood that Equation (70) applies to both cases of plane deformation in finite slabs and purely planar deformation in infinite slabs by the coefficient replacements described above.) The familiar biharmonic equation,

$$\phi_{XXXX} + 2\phi_{XXYY} + \phi_{YYYY} = -2G \frac{(1+\nu)}{(1-\nu)} \alpha T \nabla^2 (\delta T) , \quad (94)$$

is readily obtained from the scalar stress potential equation by invoking the isotropic material constants which appeared in Equations (72)-(76) for the case of "plain strain" isotropic media.

It is by now apparent that the compliances which are needed in 2-D thermoelastic computations on the X-Y plane must first be transformed to the laboratory frame in 3-D and then reduced to 2-D by elimination of the rows and columns corresponding to indices $m, n = 4, 5$ as shown schematically below:

$$s = \begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} \\ s_{21} & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} \\ s_{31} & s_{32} & s_{33} & s_{34} & s_{35} & s_{36} \\ s_{41} & s_{42} & s_{43} & s_{44} & s_{45} & s_{46} \\ s_{51} & s_{52} & s_{53} & s_{54} & s_{55} & s_{56} \\ s_{61} & s_{62} & s_{63} & s_{64} & s_{65} & s_{66} \end{pmatrix} \rightarrow \begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{16} \\ s_{21} & s_{22} & s_{23} & s_{26} \\ s_{31} & s_{32} & s_{33} & s_{36} \\ s_{61} & s_{62} & s_{63} & s_{66} \end{pmatrix} \quad (95)$$

The stress, strain, and displacement variables are thus computed in this TECATE code version as follows:

- (i) The stress potential Equation (70) is solved according to the numerical methods which are described in Appendix 1.

- (ii) The stresses $\sigma_1, \sigma_2, \sigma_6$ are obtained by numerical differentiation of the solutions for ϕ which were indicated in (i) above.
- (iii) σ_3 is evaluated from Equation (78) in the case of purely planar deformation.
- (iv) $\epsilon_1, \epsilon_2, \epsilon_6$ are evaluated from Equation (57), and $\epsilon_3 = \epsilon_4 = \epsilon_5 = 0$.
- (v) The displacement components u_1, u_2 are obtained by numerical quadrature integrations which are applied to Equation (42) as described in Appendix 1.

The method of numerical solution for the fourth-order stress potential equation mentioned in (i) above can be briefly sketched. A second-order-accurate finite difference method is utilized on a twenty-five point stencil. The analysis of local truncation errors in this PDE solution method are given in Appendix 1. As in the solution of the heat equation, Equation (70) is transformed onto the unit square according to the transformations given in Equations (3)-(6). On the domain of the unit square, Equation (70) becomes

$$A_{40}\phi_{xxxx} + A_{31}\phi_{xxxy} + A_{22}\phi_{xxyy} + A_{13}\phi_{xyyy} + A_{04}\phi_{yyyy} =$$

$$A_{20}(\delta T)_{xx} + A_{11}(\delta T)_{xy} + A_{02}(\delta T)_{yy} \quad (96)$$

The indices of A_{ij} in Equation (96) correspond notationally to the number of x and y differentiations, respectively, which appear in the stress potential and/or temperature derivative terms that multiply onto the coefficients A_{ij} . The factors A_{ij} are defined by:

$$A_{40} = \{ s_{22} + 2s_{26} \cdot \cot \alpha + (2s_{12} + s_{66}) \cot^2 \alpha +$$

$$2s_{16} \cdot \cot^3 \alpha + s_{11} \cot^4 \alpha \} / (\text{WIDTH})^4 \quad (97)$$

$$A_{31} = -2 \left\{ s_{26} + (2s_{12} + s_{66}) \cdot \cot \alpha + 3s_{16} \cot^2 \alpha + 2s_{11} \cot^3 \alpha \right\} / (WIDTH^3 \cdot HT) \quad (98)$$

$$A_{22} = \left\{ (2s_{12} + s_{66}) + 6s_{16} \cdot \cot \alpha + 6s_{11} \cot^2 \alpha \right\} / (WIDTH^2 \cdot HT^2) \quad (99)$$

$$A_{13} = -2 \left\{ s_{16} + 2s_{11} \cdot \cot \alpha \right\} / (WIDTH \cdot HT^3) \quad (100)$$

$$A_{04} = s_{11} / HT^4 \quad (101)$$

$$A_{20} = - \left\{ \alpha_2 + \alpha_6 \cdot \cot \alpha + \alpha_1 \cdot \cot^2 \alpha \right\} / WIDTH^2 \quad (102)$$

$$A_{11} = \left\{ \alpha_6 + 2\alpha_1 \cdot \cot \alpha \right\} / (WIDTH \cdot HT) \quad (103)$$

$$A_{02} = - \alpha_1 / HT^2 \quad (104)$$

Equation (96) is the PDE which is solved for the unknown potential ϕ on the unit square with the use of the dynamic ADI method in the TECATE code. The boundary conditions which ϕ is required to satisfy for free surface problems are given by

$$\phi = 0 \quad (105)$$

$$\partial \phi / \partial n = 0 \quad (106)$$

where $\hat{n}$ is the unit outer normal to the unit square. (Although clamped boundary conditions are not considered in the present TECATE code version, they can be addressed with an appropriate displacement formulation (which has also been tested in the course of this work) if/when such needs arise in the future.)

II. TECATE CODE VALIDATIONS FOR THERMOELASTIC STRESS EFFECTS

In view of the potentially complex distributions of temperature, stress, strain, and material displacements which can occur in practical applications, the TECATE code has been validated against: (i) classic thermal stress problems in thin plates which have analytic solutions in 2-D, and (ii) some newly formulated test examples which have known analytic solutions but which provide more demanding tests of convergence properties in thermal stress codes. In parallel with the TECATE code computations we have also benchmarked a totally dissimilar set of heat transfer and thermal stress codes to these problems with known analytic solutions. (The alternatively benchmarked codes^(11,12) were originally designed for orthotropic solids in applications of a much different scope than the intended applications of the TECATE code. Intercomparisons of the TECATE code results and the alternative thermal stress code results were also found to be in a reasonable agreement for a set of anisotropic material problems for which analytic solutions do not exist.) The objectives in this dual code benchmarking effort were to substantiate that: (i) accurate numerical solutions are in fact attained, (ii) high levels of computational efficiency and economy are attained, (iii) the numerical grid and accuracy convergence properties of the TECATE code agree with theoretical expectations, and (iv) the TECATE code is relatively easy to use effectively. In addition to describing code validation features, the problem discussions which follow immediately below are also intended to familiarize many readers with the basic nature and modeling of thermal stress effects in crystal systems.

A. CLASSIC 2-D THERMOELASTIC TEST PROBLEMS WITH ANALYTIC SOLUTIONS

1. Thin Plate Problem with a Polynomial Source Function

We consider first a plate of material which has a constant thickness $HT = 1$, and which is completely free of surface tractions. Analytic solutions for stress, strain, and displacement fields can be obtained in this test problem for a variety of temperature deviation functions $\delta T(x,y)$ in Equation (96). We consider a nominally rectangular plate which is taken

to be an infinite strip in the x and z co-ordinate directions, as shown in Figure 9. The temperature deviation function is given by

$$\delta T = 4y(1 - y) - \langle T \rangle \quad , \quad (107)$$

where $\langle T \rangle = \int_0^1 T(x, y) dy = \int_0^1 4y(1-y) dy = \frac{2}{3}$ is the average temperature.*

For the purpose of analytic solution, the 2-D stress potential Equation (96) reduces to

$$\begin{aligned} s_{22}^{\phi}{}_{xxxx} - 2s_{26}^{\phi}{}_{xxxy} + (2s_{12}^{\phi} + s_{66}^{\phi})\phi_{xxyy} - 2s_{16}^{\phi}{}_{xyyy} + s_{11}^{\phi}{}_{yyyy} = \\ -\alpha_2(\delta T)_{xx} + \alpha_6(\delta T)_{xy} - \alpha_1(\delta T)_{yy} \end{aligned} \quad (108)$$

Because ϕ and δT are independent of x, Equation (108) reduces to

$$s_{11}^{\phi}{}_{yyyy} = \alpha_1(\delta T)_{yy} \quad (109)$$

Figure 9. Schematic Representation of Thin Plate Problem which can be Solved Analytically as Well as Numerically.

*The analysis which follows can be carried out for much more general functions of $\delta T(x, y)$; the details of the analytic developments become more tedious, however, as increasingly general functions of x and y are considered.

subject to the boundary conditions

$$\phi(x,y) = \frac{\partial \phi(x,y)}{\partial y} = 0 \quad \text{at } y = 0 \text{ and } y = 1 \quad (110)$$

(Notice that the argument x has been retained for the sake of consistency.)

It is readily verified that the solution

$$\phi(x,y) = \frac{1}{3} (\alpha_1/s_{11}) y^2(1-y)^2 \quad (111)$$

satisfies Equations (109) and (110).

From Equations (67a)-(67c) it follows that the stresses in this example are given by

$$\sigma_{xx} = -(\alpha_1/s_{11})(4y(1-y) - \frac{2}{3}) \quad (112)$$

and

$$\sigma_{yy} = \sigma_{xy} = 0 \quad (113)$$

Material strains are obtained from Equations (107) and (112) according to Equation (52) and are found to be

$$\epsilon_{xx} = s_{11}\sigma_{xx} + \alpha_1\delta T = 0 \quad (114)$$

$$\epsilon_{yy} = s_{12}\sigma_{xx} + \alpha_2\delta T = (\alpha_2 - \alpha_1 s_{12}/s_{11})(4y(1-y) - \frac{2}{3}) \equiv \epsilon_{yy}(y) \quad (115)$$

$$\epsilon_{xy} = \frac{1}{2}(s_{16}\sigma_{xx} + \alpha_6\delta T) = \frac{1}{2}(\alpha_6 - \alpha_1 s_{16}/s_{11})(4y(1-y) - \frac{2}{3}) \equiv \epsilon_{xy}(y) \quad (116)$$

The relationships between strains ϵ_{ij} and the displacement vector (u,v) in Equation (42) are

$$\epsilon_{xx} = \frac{\partial u}{\partial x} \quad (117)$$

$$2\epsilon_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \quad (118)$$

$$\epsilon_{yy} = \frac{\partial v}{\partial y} \quad (119)$$

Noting that ϵ_{xx} , ϵ_{xy} , and ϵ_{yy} are independent of x , integration of Equation (117) with respect to x and of Equation (119) with respect to y yields

$$u(x,y) = (x - x_0)\epsilon_{xx} + u(x_0,y) \quad (120)$$

and

$$v(x,y) = \int_{y_0}^y \epsilon_{yy}(\eta) d\eta + v(x,y_0) \quad (121)$$

The arguments $x = x_0$, $y = y_0$ in Equations (120) and (121) define the arbitrary co-ordinates at which displacements are taken to be zero. The specific relationships which are implemented in the TECATE code are*

$$x_0 = y_0 = \frac{1}{2} \quad (122)$$

It remains to determine $u(x_0,y)$ and $v(x,y_0)$; for this, Equation (118) is integrated with respect to y to give

$$u(x_0,y) = 2 \int_{y_0}^y \epsilon_{xy}(\eta) d\eta - \int_{y_0}^y v_x(x_0,\eta) d\eta \quad (123)$$

*That is, the reference point $(\frac{1}{2}, \frac{1}{2})$ is taken to be the center of the unit square upon which the slab is mapped.

and with respect to x to give

$$v(x, y_0) = 2\varepsilon_{xy}(y_0)(x-x_0) - \int_{x_0}^x u_y(\xi, y_0) d\xi \quad (124)$$

One can note that the constants $u(x_0, y_0)$ and $v(x_0, y_0)$ do not appear in Equations (123) and (124) because they both vanish due to our choice of the point (x_0, y_0) . Finally, it remains to determine the last term in Equations (123) and (124). This is achieved by differentiating Equation (120) with respect to y and integrating the results from x_0 to x to obtain

$$\int_{x_0}^x u_y(\xi, y_0) d\xi = \frac{(x-x_0)^2}{2} \frac{\partial \varepsilon_{xx}(y_0)}{\partial y} + (x-x_0) u_y(x_0, y_0) \quad (125)$$

Similarly, by differentiating Equation (121) with respect to x and integrating from y_0 to y , it follows that

$$\int_{y_0}^y v_x(x_0, \eta) d\eta = v_x(x_0, y_0) \cdot (y-y_0) \quad (126)$$

One can choose without loss of generality $v_x(x_0, y_0) = 0$, and note that $u_y(x_0, y_0) = 2\varepsilon_{xy}(x_0, y_0)$. The use of Equations (114)-(116) and (122) in Equations (120) and (121) leads to the following expressions for the displacements in this example:

$$u(x, y) = -\frac{4}{3} \left(\alpha_6 - \frac{\alpha_1 s_{16}}{s_{11}} \right) y \left(y - \frac{1}{2} \right) (y - 1) \quad (127)$$

and

$$v(x, y) = -\frac{4}{3} \left(\alpha_2 - \frac{\alpha_1 s_{12}}{s_{11}} \right) y \left(y - \frac{1}{2} \right) (y - 1) \quad (128)$$

As a final note, the displacement in the x-direction (see Equation (127)) is zero in isotropic media. Although there has been no assumption that isotropic plane strain obtains in the x-direction in addition to the z-direction, this, in fact, turns out to be the case in a practical sense because the temperature variation δT and the boundary conditions are independent of x as well as of z. (Recall the conditions for purely planar deformation which were discussed above.)

2. A Comparison of Numerical and Analytic Results for Thin Plates of Isotropic YAG-like Crystals in Plane Strain*

In order to simulate a semi-infinite strip, this basic test problem is solved by the TECATE code as a 1 x 5 slab cross-section in plane strain. Except for s_{66} , the material properties of YAG are taken from Appendix 3; the non-zero material constants are:

$$\begin{aligned} s_{11} = s_{22} = s_{33} &= 3.59 \times 10^{-13} && \text{cm}^2/\text{dyne} \\ s_{12} = s_{13} = s_{23} &= -0.9 \times 10^{-13} && \text{cm}^2/\text{dyne} \\ s_{66} = 2(s_{11} - s_{12}) &= 8.98 \times 10^{-13} && \text{cm}^2/\text{dyne} \quad (129) \\ \alpha_1 = \alpha_2 = \alpha_3 &= 6.96 \times 10^{-6} && (\text{K})^{-1} \end{aligned}$$

Figures 10-13 present isocontour plots of the computed stresses and material displacements. The displacements are plotted as displaced grid mesh co-ordinates on a 65 x 33 grid mesh. An arbitrary scaling of displacement variables has been invoked for purposes of graphing. The TECATE solutions in the center of the domain (at $x = 2.5$) correspond to the infinite slab solutions which were obtained analytically in Equations (107)-(128). Comparisons of the TECATE solutions with the exact analytic results yield the following observations:

*A YAG-like isotropic crystal is formulated by letting $s_{66} = 2(s_{11} - s_{12}) = 8.98 \times 10^{-13} \frac{\text{cm}^2}{\text{dyne}}$ rather than the measured value of $8.69 \times 10^{-13} \frac{\text{cm}^2}{\text{dyne}}$.

Figure 10. Isocontour Plot of the Computed Stress σ_{xx} for an Isotropic Thin Plate in Plane Strain with Polynomial Source Function.

Figure 11. Isocontour Plot of the Computed Stress σ_{xy} for an Isotropic Thin Plate in Plane Strain with Polynomial Source Function.

Figure 12. Isocontour Plot of the Computed Stress σ_{yy} for an Isotropic Thin Plate in Plane Strain with Polynomial Source Function.

Figure 13. Deformed Material Grid for an Isotropic Thin Plate in Plane Strain with Polynomial Source Function.

- (i) The TECATE stress potential solutions are essentially analytic near the vertical center line. This result was expected because the leading terms in the local truncation error analysis for the discretization used in TECATE are proportional to sixth-order derivatives of ϕ , which are identically zero when the PDE solution depends only upon the y -variable.
- (ii) TECATE-computed values for $\sigma_{yy} \equiv \sigma_2$ and $\sigma_{xy} \equiv \sigma_6$ are zero to within computational noise (many significant figures) in the center of the domain, in agreement with theory. Non-zero values are obtained for σ_{yy} and σ_{xy} near the ends of the domain at $x = 0$ and $x = 5$, as expected. Comparisons of the TECATE solutions with alternative thermal stress code solutions away from the central region indicate close agreement between the independent code results.
- (iii) TECATE-computed values of $\sigma_{xx} \equiv \sigma_1$ agree with the analytically computed values to within accuracies of $O(h^4)$ at interior points of the domain and to within $O(h^2)$ at the domain boundaries. We recall that computed stresses are obtained by $O(h^4)$ - and $O(h^2)$ -accurate discretizations of the numerical solutions of ϕ at interior and boundary mesh points, respectively.
- (iv) The term "relative error" is defined in this work as the maximum magnitude of the quotient of the exact solution minus the numerical solution, divided by the exact solution. The ratio of relative errors in TECATE solutions for σ_{xx} in this example on a 17×17 grid, vis à vis relative errors on a 9×9 grid, confirm that the numerical solutions at interior points and at boundary points do in fact converge at the theoretically deduced magnitudes of $O(h^4)$ and $O(h^2)$, respectively. TECATE solutions of this problem on a 35×17 (x by y) grid mesh yield relative errors which are essentially identical to the relative errors in the solutions obtained on a 17×17 grid mesh, indicating that the numerical error is incurred entirely in the y -discretization for an adequate number of x -zones--consistent with the constancy of solutions in the x -direction.

- (v) TECATE-computed values of ϵ_{xy} are zero to within computational noise in the central slab region. Computed values of ϵ_{xx} and ϵ_{yy} are analytic on the interior mesh points of the domain and are $O(h^2)$ -accurate at the top and bottom boundaries, in agreement with the numerical formulations of the strains.
- (vi) TECATE solutions of the displacements are analytic to within computational noise at interior grid points and are significantly more accurate than $O(h^2)$ at the boundaries. These results are consistent with the fourth-order-accurate quadrature formulae which are used at interior points and the third-order-accurate quadrature formulae which are used in displacement calculations at boundaries.

3. Non-Thin Plate Problem for Isotropic YAG-like Crystals with a Trigonometric Source Function

The polynomial solutions which were considered in the previous example serve well as initial code benchmarks. More demanding analytical tests of the error properties of thermal stress codes are provided by problem solutions which can not be represented by strictly polynomial functions. We formulate next a set of problems on a 1×1 domain with known trigonometric solutions. For an isotropic material in "plane strain" it can be shown that the solution $\phi(x,y) = (1 - \cos 2\pi x)(1 - \cos 2\pi y)$ satisfies the biharmonic Equation (94) and the boundary conditions given by Equations (105)-(106) for the following thermal source function:

$$\delta T(x,y) = (2\pi)^2 \left(\frac{1-\nu}{\alpha E} \right) \{ 2 \cos 2\pi x \cos 2\pi y - \cos 2\pi x - \cos 2\pi y \} . \quad (130)$$

The average temperature $\langle T \rangle$ is zero in this example. The stresses obtained from Equations (67a)-(67c) are

$$\sigma_{xx} = (2\pi)^2 (1 - \cos 2\pi x) \cos 2\pi y \quad (131a)$$

$$\sigma_{yy} = (2\pi)^2 \cos 2\pi x (1 - \cos 2\pi y) \quad (131b)$$

$$\sigma_{xy} = -(2\pi)^2 \sin 2\pi x \sin 2\pi y \quad (131c)$$

The resultant strains are

$$\epsilon_{xx} = (2\pi)^2 \left(\frac{1+\nu}{E} \right) \cos 2\pi x (\cos 2\pi y - 1) \quad (132a)$$

$$\epsilon_{yy} = (2\pi)^2 \left(\frac{1+\nu}{E} \right) \cos 2\pi y (\cos 2\pi x - 1) \quad (132b)$$

$$\epsilon_{xy} = -(2\pi)^2 \left(\frac{1+\nu}{E} \right) \sin 2\pi x \sin 2\pi y, \quad (132c)$$

and the displacements are given by

$$u(x,y) = 2\pi \left(\frac{1+\nu}{E} \right) \sin 2\pi x (\cos 2\pi y - 1) \quad (133a)$$

$$v(x,y) = 2\pi \left(\frac{1+\nu}{E} \right) \sin 2\pi y (\cos 2\pi x - 1) \quad (133b)$$

Figures 14-19 present TECATE solutions for the temperature, stress potential, stresses, displacements, and displaced grid mesh, respectively, for YAG crystals in this test problem. It is interesting to note that the material displacements at the boundaries are zero to within rigid body displacements even though free surface boundary conditions were applied. This result is thus somewhat paradoxical because the solutions of the free surface boundary value problem in fact describe a clamped boundary. Comparisons of the TECATE-computed stress potential to the analytical results above indicate that a maximum error of approximately 0.1% is incurred in the center of the domain for a 65 x 65 computational grid mesh. This is consistent with the $O(h^2)$ error magnitude evaluated from theoretical analysis. (Recall that solution derivatives of higher order which appear in coefficients of the local truncation error terms are non-zero; these coefficients can in fact become quite large for the non-polynomial solution considered in this example.) A sequence of calculations on grid meshes of 9 x 9, 17 x 17, 33 x 33, and 65 x 65 confirms that the error diminishes almost exactly as $O(h^2)$. The error properties of computed stresses and displacements are

Figure 14. Isocontour Plot of the Temperature for an Isotropic Slab with Harmonic Source Function.

Figure 15. Isocontour Plot of the Computed Stress Potential for an Isotropic Slab with Harmonic Source Function.

Figure 16. Isocontour Plot of the Computed Stress σ_{xx} for an Isotropic Slab with Harmonic Source Function.

Figure 17. Isocontour Plot of the Computed Stress σ_{yy} for an Isotropic Slab with Harmonic Source Function.

Figure 18. Isocontour Plot of the Computed Stress σ_{yy} for an Isotropic Slab with Harmonic Source Function.

Figure 19. Deformed Material Grid for an Isotropic Slab with Harmonic Source Function.

similar in their general features to those mentioned in the previous example.

4. Anisotropic Results. Thin Crystalline KDP Plate with Polynomial Source Function.

We consider in this example material slabs which have been cut in arbitrary orientations relative to the crystal axes (a,b,c). KDP crystals are tetragonal and are represented in their conventional frame of orthogonal co-ordinate axes (x_1, x_2, x_3) in Figure 20. The material properties in this conventional co-ordinate frame are (from Appendix 3):

$$\begin{aligned}
 s_{22} &= s_{11} = 1.78 \times 10^{-12} \text{ cm}^2/\text{dyne} \\
 s_{12} &= -3.8 \times 10^{-13} \\
 s_{23} &= s_{13} = -7.1 \times 10^{-13} \\
 s_{33} &= 2.03 \times 10^{-12} \\
 s_{55} &= s_{44} = 8.1 \times 10^{-12} \\
 s_{66} &= 1.64 \times 10^{-11}
 \end{aligned} \tag{134}$$

Figure 20. Potassium dihydrogen phosphate (KDP), a tetragonal crystal, class $\overline{4}2m$.

$$\alpha_1 = \alpha_2 = 2.49 \times 10^{-5} (^\circ\text{K})^{-1}$$

$$\alpha_3 = 4.40 \times 10^{-5}$$

$$k_1 = k_2 = 1.86 \times 10^5 \text{ ergs/cm sec } ^\circ\text{K}$$

$$k_3 = 2.09 \times 10^5$$

The sample problems below are analyzed in simple plate orientations which are intended to illustrate both the modeling procedures and certain thermal stress effects for anisotropic crystals. The polynomial temperature source function of Equation (107) is used in these sample problems.

(a) Conventional Orientation

In this baseline case, the laboratory co-ordinates (X,Y,Z) are simply $X = x_1$, $Y = x_2$, and $Z = x_3$. A slab with cross-sectional dimensions of 1 x 5 in the a-b plane is considered in this 2-D computation; and the slab dimension in the Z direction is taken to be infinite. An isocontour plot of the temperature variation δT is plotted in Figure 21, and isocontours of the stress potential are plotted in Figure 22. Isocontours of the stress components are plotted in Figures 23 to 25. Grid (or material) displacements appear in Figure 26. Broken lines denote negative values in the contour plots. Grid displacements are plotted according to a scaling procedure in which the maximum magnitude of the displacement vector is scaled to a magnitude which is equal to 10% of the minimum domain length. (That is, the maximum magnitude of the vector denoted by (u, v) is equal to .1 in the present example.) It is apparent here, and it will continue to hold true, that the most radical thermoelastic stress effects occur at material boundaries. This sample problem can also be solved for non-rectangular slab cross sections. Figures 27 to 32 present results for a parallelogram slab cross-section with $\text{ANGLE} = 60^\circ$; these results are seen to follow closely the corresponding stress, strain, and displacement distributions which were obtained for the preceding rectangular slab.

Figure 21. Isocontour Plot of the Temperature for a KUP Slab with Polynomial Source Function.

Figure 22. Isocontour Plot of the Computed Stress Potential for a KUP Slab with Polynomial Source Function.

Figure 23. Isocontour Plot of Computed σ_{xx} for a KDP Slab with Polynomial Source Function.

Figure 24. Isocontour Plot of Computed σ_{xy} for a KDP Slab with Polynomial Source Function.

Figure 25. Isocontour Plot of Computed σ_{yy} for a KDP Slab with Polynomial Source Function.

Figure 26. Deformed Material Grid for a KDP Slab with Polynomial Source Function.

Figure 27. Isocontour Plot of the Computed Temperature for a KDP Slab with Non-Rectangular Cross-Section.

Figure 28. Isocontour Plot of the Computed Stress Potential for a KDP Slab with Non-Rectangular Cross-Section.

Figure 29. Isocontour Plot of the Computed Stress σ_{xx} for a KDP Slab with Non-Rectangular Cross-Section.

Figure 30. Isocontour Plot of the Computed Stress σ_{xy} for a KDP Slab with Non-Rectangular Cross-Section.

Figure 31. Isocontour Plot of the Computed Stress σ_{yy} for a KDP Slab with Non-Rectangular Cross-Section.

Figure 32. Deformed Material Grid for a KDP Slab with Non-Rectangular Cross-Section.

(b) Rectangular KDP Slab Cut at 30° to the Crystal Axes (a,b)

We consider next a problem in which the 2-D cross section of a rectangular KDP slab is cut so that the slab cross-sectional faces subtend angles of 30° with the crystal axes (a,b). The slab is assumed to be infinite in the axial (Z) direction. The direction cosines according to the conventions discussed previously (see Figure 6 also) are

$$\begin{aligned} a_{11} &= 0.866 & a_{12} &= 0.5 & a_{13} &= 0. \\ a_{21} &= -0.5 & a_{22} &= 0.866 & a_{23} &= 0. \\ a_{31} &= 0. & a_{32} &= 0. & a_{33} &= 1.0 \end{aligned} \quad (135)$$

Application of the tensor transformations expressed in Equations (39) and (47) upon the material properties given by Equations (134) in the conventional ("old") co-ordinate system yield the following values in the "new" co-ordinate frame which is indicated in Figure 33:

$$\begin{aligned} s_{22} &= s_{11} = 4.045 \times 10^{-12} \text{ cm}^2/\text{dyne} \\ s_{12} &= -2.645 \times 10^{-12} \\ s_{23} &= s_{13} = -7.1 \times 10^{-13} \\ s_{33} &= 2.03 \times 10^{-12} \\ s_{55} &= s_{44} = 8.1 \times 10^{-12} \\ s_{16} &= 2.6154 \times 10^{-12} \\ s_{26} &= -2.6154 \times 10^{-12} \\ s_{66} &= 7.34 \times 10^{-12} \\ \alpha_1 &= \alpha_2 = 2.49 \times 10^{-5} \text{ (}^\circ\text{K)}^{-1} \\ \alpha_3 &= 4.40 \times 10^{-5} \\ k_1 &= k_2 = 1.86 \times 10 \text{ ergs/cm sec } ^\circ\text{K} \\ k_3 &= 2.09 \times 10^5 \end{aligned} \quad (136)$$

Figure 33. A 2-D KDP Cross Section. The slab is taken to be infinite in the axial direction (normal to the plane of this page). A 30° angle is subtended between the rectangular slab faces and the crystal axes (a,b).

This rotation of old-to-new axes in the a-b crystal plane introduces non-zero values for the compliance elements s_{16} and s_{26} and leaves the thermal expansion and thermal conduction coefficients unchanged. Figures 34 to 37 present selected stress and displacement distributions for the temperature source function $T = 4Y^{New}(1 - Y^{New})$. The differences which are apparent between these results in the rotated rectangular slab and those in Figures 21 to 26 for the conventional frame are due entirely to the crystal orientations, as embodied in the alternative material properties expressed in Equations (136) and Equations (134), respectively. The results in all of these examples with δT given by the polynomial expression $4Y(1 - Y)$ agree with analytic solutions, as discussed in the sections above. We turn our attention now to more physically meaningful examples for which analytic solutions have not been generally available but which have been benchmarked successfully with alternative thermal stress codes in 2-D.

B. CRYSTALS IMMERSED IN COOLANT FLOWS

The next several examples consider helium coolant which flows over the top and bottom surfaces of selected anisotropic crystals in both co-flowing

Figure 34. Isocontour Plot of the Computed Stress σ_{xx} for a KUP Slab with its Base Surface Cut at an Angle of 30° from the a-Axis.

Figure 35. Isocontour Plot of the Computed Stress σ_{yy} for a KUP Slab with its Base Surface Cut at an Angle of 30° from the a-Axis.

Figure 36. Isocontour Plot of the Computed Stress σ_{yy} for a KDP Slab with its Base Surface Cut at an Angle of 30° from the a-Axis.

Figure 37. Deformed Material Grid for a KDP Slab with its Base Surface Cut at an Angle of 30° from the a-Axis.

and counter-flowing configurations (see Figures 1a and 1b). The helium temperatures at the upstream and downstream corners of the crystal are treated as given quantities. The end surfaces of the simulated slab are taken to be insulated. (Numerous other boundary conditions for the end surfaces have been computed and found to yield results which are generally similar to those discussed below.) The material stresses σ_{xx} , σ_{xy} , and σ_{yy} are of primary interest in this work due to their ultimate role in optical propagation analyses.

In order to briefly review the role of material stresses in optical propagation processes, it is useful to sketch the analytical dependence of indices of refraction upon elastic stresses in simple solids. For this we can consider an initially unstressed, optically isotropic material which becomes optically anisotropic when the material becomes stressed. The refractive index of a crystal is specified by the indicatrix, which is an ellipsoid whose coefficients B_{ij} are the components of the relative dielectric impermeability; that is,

$$B_{ij} x_i x_j = 1, \quad i, j = 1, 2, 3, \quad (137)$$

$$\text{where } B_{ij} = \kappa_0 \partial E_i / \partial U_j, \quad (138)$$

$$\kappa_0 \equiv \text{permittivity of a vacuum}, \quad (139)$$

$$\underline{E} \equiv \text{electric field vector} \quad (140)$$

$$\underline{D} \equiv \text{electric displacement vector}. \quad (141)$$

In the frame of principal axes, one can write

$$B_1 x_1^2 + B_2 x_2^2 + B_3 x_3^2 = 1, \quad (142)$$

where $B_i = \frac{1}{n_i^2}$, and n_i are principal refractive indices. It follows that

$$\Delta B_i = -\frac{2}{n_i^3} \Delta n_i. \quad (143)$$

In the case of an unstressed cubic crystal,

$$B^0(x_1^2 + x_2^2 + x_3^2) = 1 \quad , \quad (144)$$

and the indicatrix is a sphere. The refractive index is $n^0 = \frac{1}{\sqrt{B^0}}$. When a stress is applied, the indicatrix is

$$B_1 x_1^2 + B_2 x_2^2 + B_3 x_3^2 + 2B_4 x_2 x_3 + 2B_5 x_3 x_1 + 2B_6 x_1 x_2 = 1 \quad . \quad (145)$$

The change in the coefficients B_m (in the compact notation) for the photo-elastic effect is given by

$$\Delta B_m = \pi_{mn} \sigma_n \quad , \quad m, n = 1, \dots, 6 \quad , \quad (146)$$

where π_{mn} denotes the piezo-optical coefficients. It follows from Equations (143) and (146) that, to a good approximation, a uniaxial stress σ_j applied along a cube axis (denoted previously by x_j) gives refractive index changes

$$\Delta n_i = - \frac{(n^0)^3}{2} \pi_{ij} \sigma_j \quad , \quad i, j = 1, 2, 3 \quad (147)$$

The index of refraction can thus become directionally dependent when a stress σ_j is applied to the crystal. In addition to evaluations of the material stresses σ_j , optical propagation computations also require physical data for the piezo-optical coefficients π_{ij} . The matrix structures of π_{ij} for the various crystal symmetry classes are given in Reference 5. Although π_{ij} may generally resemble the corresponding compliance and elastic stiffness matrices, it is found in practice that the respective symmetry properties of π_{ij} and s_{ij} may sometimes be quite dissimilar. For example, compliance matrices s_{ij} are symmetric for all crystal classes, and piezo-optical matrices are not symmetrical in several crystal classes. With these factors in mind, we examine now some sample stress distributions in flashlamp-irradiated crystals.

1. Co-Flowing Helium Over Top and Bottom Surfaces of a Cubic YAG Crystal

Problem Parameters:

Slab dimensions are 1 cm x 5 cm. Helium film coefficients are taken to be

$$h = 4.75 \times 10^5 \frac{\text{ergs}}{\text{sec-cm}^2 \cdot ^\circ\text{K}}$$

Flashlamp power densities on the top and bottom surfaces = $2.5 \times 10^6 \frac{\text{ergs}}{\text{cm}^2 \cdot \text{sec}}$

Flashlamp absorption is assumed to be like Nd: glass with $\rho_n = 4.6 \times 10^{19}$ and $B = .7127$; $C = .1343$; $D = 1.1167$. Non-zero material properties for YAG are

$$k_{11} = k_{22} = 1.30 \times 10^6 \frac{\text{ergs}}{\text{sec-cm} \cdot ^\circ\text{K}}$$

$$\alpha_{11} = \alpha_{22} = \alpha_{33} = 6.96 \times 10^{-6} (^\circ\text{K})^{-1}$$

$$s_{11} = s_{22} = s_{33} = 3.59 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{12} = s_{13} = s_{23} = -0.9 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{66} = 8.69 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

Figures 38 and 39 present isometric and contour graphs of slab temperatures as a function of X and Y. The coolant temperature T_c at the upstream and downstream boundaries is also indicated in Figure 38. The coolant temperatures along the boundaries are assumed to vary linearly between the

Figure 38. Temperature Distribution in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 39. Isocontour Plot of the Computed Temperature in a YAG Slab with Co-Flowing Helium Coolant.

designated end values. The slab temperatures T are then computed along the surface boundaries according to the film boundary condition discussed previously. In the next stage of computations, derivatives of the computed slab temperature distribution are used to evaluate source terms for the numerical integration of the stress potential Equation (96). Material stresses, strains and displacements are then evaluated from the stress potential solutions. Figures (40)-(42) present isometric graphs of the computed stresses σ_{xx} , σ_{xy} , and σ_{yy} , respectively. Isocontour graphs of these stresses are presented in Figures (43) - (45). It is apparent that large stress variations occur predominantly at the slab boundaries. (Positive stresses represent tension, and negative stresses represent material compressions.) Maximum tensile stresses computed in this example are on the order of 10^5 Pa. Tensile yield strengths of YAG crystals are approximately 4×10^8 Pa. Material displacements are represented by the scaled displaced grid mesh co-ordinates in Figure 46. The displacements in Z are constant, and the planar X - Y grid displacements are plotted relative to the displacements at the center of the slab cross section.

2. Counter-Flowing Helium on YAG Crystal

The slab temperature pattern in this example can be seen to resemble qualitatively the temperature distributions which may occur in such disc laser systems as are indicated schematically below.

The temperature distribution for this case, which is shown in Figures 47 and 48, is skewed significantly relative to the previous example. The stresses shown in Figures 49-54 for the present case are qualitatively similar to the previously considered co-flow results. But the computed

Figure 40. σ_{xx} Computed in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 41. σ_{xy} Computed in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 42. σ_{yy} Computed in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 43. Isocontour Plot of the Computed Stress σ_{xx} in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 44. Isocontour Plot of the Computed Stress σ_{xy} in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 45. Isocontour Plot of the Computed Stress σ_{yy} in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 46. Deformed Material Grid in a Rectangular YAG Slab with Co-Flowing Helium Coolant.

Figure 47. Temperature Distribution in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 48. Isocontour Plot of Computed Temperature in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 49. σ_{xx} Computed in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 50. σ_{xy} Computed in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 51. σ_{yy} Computed in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 52. Isocontour Plot of the Computed Stress σ_{xx} in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 53. Isocontour Plot of the Computed Stress σ_{yy} in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 54. Isocontour Plot of Computed Stress σ_{yy} in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

Figure 55. Deformed Material Grid in a Rectangular YAG Slab with Counter-Flowing Helium Coolant.

strains (not shown) and the material displacements plotted in Figure 55 exhibit marked differences in this counter-flow example, vis à vis the previous results for co-flowing coolant.

3. Co-Flowing Helium on a KDP Slab. The a-b Crystal Plane is Modeled.

In order to examine distinctions which arise only from crystal symmetry properties, tetragonal KDP crystals are studied in the same co-flow coolant and flashlamp source environments as were considered in the YAG examples above. In conventional co-ordinate axes orientations, thermal conductivities have the same structure in the a-b plane of KDP as in YAG, but thermal expansion and compliance tensors have obvious structural differences in these two materials, as can be seen immediately below and in Appendix 2.

$$k_{11} = k_{22} = 1.86 \times 10^5 \frac{\text{ergs}}{\text{sec-cm}^\circ\text{K}}$$

$$\alpha_{11} = \alpha_{22} = 2.49 \times 10^{-5} (^\circ\text{K})^{-1}; \alpha_{33} = 4.4 \times 10^{-5} (^\circ\text{K})^{-1}$$

$$s_{11} = s_{22} = 1.78 \times 10^{-12} \text{ cm}^2/\text{dyne}$$

$$s_{12} = -3.8 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{13} = s_{23} = -7.1 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{33} = 2.03 \times 10^{-12} \text{ cm}^2/\text{dyne}$$

$$s_{66} = 1.64 \times 10^{-11} \text{ cm}^2/\text{dyne}$$

Figures 56-60 for the computed temperature and stress distributions in KDP with co-flowing helium coolant are qualitatively similar to the YAG results discussed in sample problem 4 above. Due to its particular crystal symmetry properties, the computed material displacements which appear for KDP in Figure 60 are nominally different than the computed material displacements in the corresponding YAG results which appeared previously in Figure 46. An analogous computation of a cross section in the b-c plane of a KDP slab with the corresponding co-flowing helium coolant orientation yielded results which resemble qualitatively -- but not completely quantitatively -- these computed results in the a-b plane of KDP. The distinctions between computed stresses and displacements in the a-b versus the b-c planes of KDP slabs are sufficiently incidental that plots of the results for the b-c plane of KDP are omitted.

4. Co-Flowing Helium on a KDP Slab Which is Cut at 30° to the a-b Crystal Axes.

By cutting the KDP crystal considered immediately above so that the new horizontal and vertical crystal surfaces subtend an angle of 30° relative to the a-b crystal axes, the non-zero material properties are given by

$$k_{11} = k_{22} = 1.86 \times 10^6 \frac{\text{ergs}}{\text{sec-cm}^2\text{-}^\circ\text{K}}$$

Figure 56. Isocontour Plot of the Computed Cross-Sectional Temperature for a KDP Slab Cut with Surfaces Parallel to the a-b Axes in Co-Flowing Helium Coolant.

Figure 57. Isocontour Plot of the Computed Stress σ_{xx} for a KDP Slab Cut with Surfaces Parallel to the a-b Axes in Co-Flowing Helium Coolant

Figure 58. Isocontour Plot of the Computed Stress σ_{xy} for a KDP Slab Cut with Surfaces Parallel to the a-b Axes in Co-Flowing Helium Coolant.

Figure 59. Isocontour Plot of the Computed Stress σ_{yy} for a KDP Slab with Surfaces Parallel to the a-b Axes in Co-Flowing Helium Coolant.

Figure 60. Deformed Material Grid for a KDP Slab Cut with Surfaces Parallel to the a-b Axes in Co-Flowing Helium Coolant.

$$\alpha_{11} = \alpha_{22} = 2.49 \times 10^{-5}; \alpha_{33} = 4.4 \times 10^{-5} (^{\circ}\text{K})^{-1}$$

$$s_{11} = s_{22} = 4.045 \times 10^{-12} \text{ cm}^2/\text{dyne}$$

$$s_{12} = -2.645 \times 10^{-12}$$

$$s_{13} = s_{23} = -7.1 \times 10^{-13}$$

$$s_{16} = -s_{26}' = 2.615 \times 10^{-12}$$

$$s_{33} = 2.03 \times 10^{-12}$$

$$s_{66} = 7.34 \times 10^{-12}$$

In addition to altering the magnitude of several non-zero compliance matrix elements from previous examples, the rotation which describes this new crystal surface orientation also introduces non-zero compliance matrix elements s_{16} and s_{26} . Whereas the temperature contours in Figure 61 are qualitatively similar to those in the previous sample problem (i.e., prior to rotation by 30°), the stress contours in Figures 62-64 exhibit distinctly skewed features due to the rotated orientation of the KDP crystal surfaces relative to the a-b axes. The material displacements in Figure 65 are qualitatively similar to, but greater in magnitude than, the displacements computed for the unrotated slab, shown previously in Figure 60.

5. Co-Flowing Helium on a KDP Slab which is cut at 30° to b-c Crystal Axes.
(This is a double rotation from the conventional x_1, x_2, x_3 axes.)

Finally, we consider the KDP crystal to be cut so that the horizontal and vertical surfaces subtend an angle of 30° to the b-c crystal axes. The material properties for this rectangular crystal are

Figure 61. Isocontour Plot of the Computed Cross Sectional Temperature for a KDP Slab with Surfaces Cut at 30° to the a-b Axes in Co-Flowing Helium Coolant.

Figure 62. Isocontour Plot of the Computed Stress σ_{xx} for a KDP Slab with Surfaces Cut at 30° to the a-b Axes in Co-Flowing Helium Coolant.

Figure 63. Isocontour Plot of the Computed Stress σ_{xy} for a KUP Slab with Surfaces Cut at 30° to the a-b Axes in Co-Flowing Helium Coolant.

Figure 64. Isocontour Plot of the Computed Stress σ_{yy} for a KUP Slab with Surfaces Cut at 30° to the a-b Axes in Co-Flowing Helium Coolant.

Figure 65. Deformed Cross-Sectional Grid for a KDP Slab with Surfaces Cut at 30° to the a-b Axes in Co-Flowing Helium Coolant.

$$k_{11} = 2.03 \times 10^5; k_{12} = -9.96 \times 10^3; k_{22} = 1.92 \times 10^5 \text{ ergs/sec-cm-}^\circ\text{K}$$

$$\alpha_{11} = 3.923 \times 10^{-5}; \alpha_{22} = 2.968 \times 10^{-5}; \alpha_{33} = 2.49 \times 10^{-5} (^\circ\text{K})^{-1}$$

$$\alpha_{12} = -1.654 \times 10^{-5} (^\circ\text{K})^{-1}$$

$$s_{11} = 2.506 \times 10^{-12} \text{ cm}^2/\text{dyne}$$

$$s_{12} = -1.248 \times 10^{-12}$$

$$s_{13} = -6.28 \times 10^{-13}$$

$$s_{16} = 5.13 \times 10^{-13}$$

$$s_{22} = 2.38 \times 10^{-12}$$

$$s_{23} = -4.63 \times 10^{-13}$$

$$s_{26} = -7.30 \times 10^{-13}$$

$$s_{33} = 1.78 \times 10^{-12}$$

$$s_{36} = 2.86 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{66} = 5.948 \times 10^{-12}$$

Several new features can be noted in the structure of the material properties for this case: (i) non-zero values have now appeared for k_{12} and α_{12} ; (ii) α_{11} is no longer equal to α_{22} ; (iii) a non-zero value has emerged for s_{36} ; and (iv) except for diagonal symmetry of the compliance matrix, individual compliance matrix elements have unequal values. The results which appear in Figures 66-70 indicate that only nominal qualitative differences--but significant quantitative distinctions--exist between temperature distributions for the co-flowing coolant configurations considered in these KDP examples. The material stresses in the b-c crystal plane of KDP in the present example exhibit the same general skewness features as those observed in modeling of the a-b crystal plane of KDP. The material displacements indicated in Figure 70 differ substantially, however, from the displacements which appeared in Figure 65 for a corresponding rectangular cross section in the a-b plane of KDP.

C. SUMMARY OF SAMPLE PROBLEMS

The sample problems above were selected in order to examine both separately and collectively those macroscopic effects which may be associated with (i) thermal flow environments, (ii) anisotropies which are intrinsic in crystalline structure, per se, and (iii) anisotropies which emerge primarily as a function of crystal shape and orientation.

Sample problems 1-4 of section A considered analytically specified temperature distributions. Problems 1, 2, and 3 examined markedly different polynomial and trigonometric temperature distribution functions in the same cubic material, YAG. Problem 4 in Section A considered KDP, a tetragonal crystal, versus the cubic crystal YAG with the same polynomial temperature

Figure 66. Isocontour Plot of the Computed Cross Sectional Temperature for a KDP Slab with Surfaces Cut at 30° to the b-c Axes in Co-Flowing Helium Coolant.

Figure 67. Isocontour Plot of the Computed Stress σ_{xx} for a KDP Slab with Surfaces Cut at 30° to the b-c Axes in Co-Flowing Helium Coolant

Figure 68. Isocontour Plot of the Computed Stress σ_{xy} for a KUP Slab with Surfaces Cut at 30° to the b-c Axes in Co-Flowing Helium Coolant.

Figure 69. Isocontour Plot of the Computed Stress σ_{yy} for a KUP Slab with Surfaces Cut at 30° to the b-c Axes in Co-Flowing Helium Coolant.

Figure 70. Deformed Cross-Sectional Grid for a KUP Slab with Surfaces Cut at 30° to the b-c Axes in Co-Flowing Coolant.

distribution as in sample problems 1 and 2. Problem 4 also examined the effects of (i) crystal shapes in rectangular versus non-rectangular cross sections of KDP in the conventional axis frame, and (ii) crystal orientations for rectangular cross sections with crystal faces both parallel and rotated by 30° relative to the a-b crystal axes.

Problems 1-5 in section B above considered rectangular YAG and KDP crystal slabs immersed in both co-flowing and counter-flowing helium coolant environments. Sample problems 1 and 2 in section B examined the effects of alternative temperature distributions associated with co-flow versus counter-flow coolant conditions in YAG crystals. Sample problem 3 considered a KDP crystal in co-flowing helium over the top and bottom crystal surfaces; the horizontal and vertical crystal surfaces were taken to be parallel to the conventional a-b crystal axes. Results of this problem were cross-compared with results of both sample problem 4 in section A for KDP in its conventional axis frame with a polynomial temperature distribution and sample problem 1 in section B for YAG in co-flowing helium. Sample problems 3-5 of section B considered alternative surface orientations of KDP crystals in co-flowing helium coolant. Purely planar deformations have been considered in these examples. General planar deformations will be considered for trigonal and perhaps other crystal systems in a forthcoming report which presents the 2 1/2-D formulation based upon two stress potentials in two spatial variables. (Also see Appendix 1.)

III. TECATE CODE DESCRIPTIONS AND SAMPLE WORK SESSIONS

The TECATE code solves two basic problems numerically: (i) it computes the solution to the steady state heat equation (2); and (ii) it computes solutions to the stress potential Equation (70) and the derived stresses, strains, and material displacements. The user can elect to solve these two problems either individually or both together, in conjunction with each other (see Figure 71).

A. GENERAL CODE PARAMETERS

The three basic modes of operation are selected by using the following input parameter designations:

IPROB = 1	Computes the temperature only
IPROB = 2	Computes the stress potential and the derived stresses, strains, and material displacements
IPROB = 0	Computes both the temperature and the stress potential; the source term of the stress potential equation is evaluated from the computed temperature distribution. This is the default option.

A second problem parameter JPROB defines additional solution options in conjunction with IPROB as follows.

For IPROB = 0 or 1, JPROB selects the heating sources as

JPROB = 0, Flashlamp sources are defined by Equations (21) - (29). Source power densities in Equation (29) are defined by PWRBL at the slab's bottom left corner, PWRBR at the bottom right corner, PWRTL at the top left corner, and PWTRR at the top right corner. The power source densities are assumed to be spatially linear along the top and bottom slab surfaces.

JPROB = 1, Polynomial source function of maximum degree 8:

$$Q(x,y) = \sum_{0 \leq r+s \leq 8} C_{rs} x^r y^s$$

For IPROB = 2, JPROB selects temperature distributions for stress potential sources as:

JPROB = 0, Reads input data file TEMPS

JPROB = 1, Polynomial source function of maximum degree :

$$T(x,y) = \sum_{0 \leq r+s \leq 8} C_{rs} x^r y^s$$

Stress computations utilize temperature deviations $\delta T = T - T_{ref}$ according to the parameters :

ITREF = 0, Default option which uses $T_{ref} = \langle T \rangle$, the spatially averaged temperature which is computed internally.

ITREF = 1, Uses an arbitrary reference temperature TREF which is read in the input file HOPS.

The 2-D slab geometry considered by TECATE was indicated schematically in Figure 2. The code parameters WIDTH and HT must be assigned strictly positive values. The parameter ANGLE represents α in degrees; this angle is restricted to be greater than zero but less than or equal to 90. The default value is ANGLE = 90°.

Figure 71. Schematic Representation of the TECATE Code.

The computational grid was indicated schematically in Figure 3. The grid spacing is uniform in x and y and is specified by indicating the number of grid columns, NCOL, and the number of grid rows, NROW. Both NCOL and NROW must be ≥ 5 . There is also a maximum number of grid columns and rows determined by the size of the arrays in TECATE. Currently NCOL and NROW must be ≤ 81 . The modification required to run with larger grids is quite simple.

The maximum number of iterations of the dynamic ADI method in TECATE is specified by the parameter NLOOP. The default value for NLOOP of 250 should be quite sufficient for most applications. The number of iterations actually used depends upon the rate of convergence of the relative error norm (which is defined at the n^{th} iteration as the ratio $\|u^n - u^{n-1}\| / \|u^n\|$) and which is required not to exceed the parameter REDN. The default value for REDN is 10^{-9} , although much larger values (such as 10^{-6}) usually suffice.

For large computational grids, the amount of output generated by TECATE can become voluminous if the solution calculated at each grid point is printed. To alleviate this problem, a user may indicate that solution values are to be output at every k^{th} column and l^{th} row only. The values of k and l are specified by NEACHC and NEACHR respectively. The default value for each of these parameters is 1; i.e., each solution is to be printed out at every grid point.

B. TEMPERATURE CALCULATION PARAMETERS

The thermal conductivities k_{11} , k_{12} , and k_{22} in the steady state heat equation (2) are specified by the parameters CONU11, CONU12 and CONU22, respectively, and should be in the units power/length-degree. Before discussing the nature of the source function Q , we first describe the boundary conditions.

For each side of the domain Ω , three types of boundary conditions are considered (the outward unit normal to $\partial\Omega$ is denoted by $\underline{m}$):

- (i) Dirichlet; $T = f$, where f is a given linear function
- (ii) Natural condition; $(\underline{k} \cdot \underline{\nabla} T) \cdot \underline{\hat{m}} = \lambda$, for constant λ
- (iii) Film condition; $(\underline{k} \cdot \underline{\nabla} T) \cdot \underline{\hat{m}} = h(T_c - T)$ where T_c is a given linear function (the coolant temperature) and h is a positive constant.

For each side of the domain Ω , the user must specify one of the boundary conditions described above. The condition at the left boundary is specified using the parameter NEUML, where

NEUML = 0, Dirichlet condition (default)
 NEUML = 1, Film condition
 NEUML = 2, Natural condition

Similarly, the conditions for the right, top and bottom boundaries are specified by the parameters NEUMR, NEUMT, and NEUMB. In order to assure the existence and uniqueness of PDE solutions, it is essential that all four sides are not assigned the natural boundary condition of type (ii) above. (Note that (iii) is of the type (ii) if $h = 0$.) For a Dirichlet condition, the temperature T is taken to be spatially linear on each side, and the boundary temperatures are defined by specifying T at the four corners of the domain. In the same way, the coolant temperature T_c is given by specifying T_c at the four corners. The parameters used to assign these corner values are indicated below:

UBL, T at the bottom left corner	UAMBBL, T_c at the bottom left corner
UBR, T at the bottom right corner	UAMBBR, T_c at the bottom right corner
UTL, T at the top left corner	UAMBTL, T_c at the top left corner
UTR, T at the top right corner	UAMBTR, T_c at the top right corner

For example, if there is a Dirichlet condition on the top boundary NEUMT = 0, the temperature along that side is defined by assigning UTL and UTR the appropriate values. Similarly, if there is a film condition on the top boundary NEUMT = 1, the coolant temperature is defined by assigning UAMBTL and UAMBTR the appropriate values. The default for all of these parameters is 0. Finally, the constants λ and h used in the natural and film boundary conditions, are specified on the left, right, top and bottom sides by the parameters FLMCFL, FLMCFR, FLMCFT, and FLMCFB which have default values of 0.

C. STRESS CALCULATION PARAMETERS

The basis for the derivation of the 2-D stress potential equation is the generalized Hooke's law which relates the strains to the stresses and temperature variation according to Equation (59b). The constants s_{mn} are the compliance matrix elements in compact notation, and α_m are the thermal expansion coefficients defined according to Equations (51).

D. SUBROUTINE DESCRIPTIONS

BRAIN	The executive routine for the DADI method which is used to solve the discretized steady state heat equation and the discretized stress potential equation. Either the heat equation or the potential equation is solved depending upon the subroutine argument.
RATIO	Computes the test parameter and convergence factor used in the DADI strategy and some other relevant norms.
PRINTIT	Writes DADI convergence history to the output file.
MARCH	Performs a single DADI iteration consisting of two ADI steps and a single ADI step for bookkeeping purposes.
RESH	Calculates the residual of the discretized heat equation.
RESS	Calculates the residual of the discretized potential equation.
SOLTDX	Decomposes and solves a tri-diagonal system of linear equations. Specifically, it performs an x-sweep in an ADI solution step of the discretized heat equation.
SOLTDY	Performs the same function as SOLTDX except that we now sweep along y instead of x.
SOLPDX	Decomposes and solves a penta-diagonal system of linear equations. Specifically, it performs an x-sweep in an ADI solution step of the discretized potential equation.
SOLPDY	Performs the same function as SOLPDX except that we now sweep along y instead of x.
COEFH	Computes and scales the new coefficients of the heat equation on the unit square. This transformation from the parallelogram to the unit square should be transparent to the user.
COEFS	Computes and scales the new coefficients of the potential equation on the unit square.

MXELMH Computes and stores the elements of the tri-diagonal matrices corresponding to the x and y-sweeps in an ADI solution step for the discretized heat equation.

MXELMS Computes and stores the elements of the penta-diagonal matrices corresponding to the x and y-sweeps in an ADI solution step for the discretized potential equation.

SEIBCSH Initializes the solution vector and associated working vectors of the potential equation to zero everywhere.

LOADHQ Scales and loads the heat equation source vector which may have been computed elsewhere.

CHSRCD Computes the heat equation source vector by numerically differencing a polynomial solution.

E. FIRST SAMPLE WORK SESSION

The thin plate stress problem with a polynomial heat source function which was considered as the first test problem in section IIA above serves also as the sample problem in this work session. (The results of this problem were discussed previously in the context of Equations (107)-(129)).

1. Input

The TECATE input file name is HOPS. The input data for this sample problem is provided in the namelist file immediately below, followed by a brief discussion of the selected input parameter values.

```

iprob = 2
jprob = 1
$
ncol = 65
nrow = 33
width = 5.
ht = 1.
angle = 90.
neachc = 8
neachr = 4
redn = 1.e-7
nloop = 250
jextrp = 4
itref = 1
tref = .66666667
iso = 0
alph11 = 6.96e-6
alph22 = 6.96e-6
alph33 = 6.96e-6
alph12 = 0.
s11 = 3.59e-13
s12 = -.9e-13
s13 = -.9e-13
s16 = 0.
s22 = 3.59e-13
s23 = -.9e-13
s26 = 0.
s33 = 3.59e-13
s36 = 0.
s66 = 8.98e-13
ngeo = 1
integ = 4
c01 = 4.
c02 = -4.
$

```

The parameter JEXTRP = 4 applies fourth degree polynomial extrapolations in boundary condition discretizations. This is the maximum value presently permitted for JEXTRP; a quintic extrapolation will be available in future code versions. The default value of ISO = 0 signals that thermal expansion coefficients ALPH11, ... , etc. and compliance matrix elements s11, ... , etc., will be read into the code on a matrix element-by-matrix element basis, which is the required option for anisotropic materials. For isotropic materials, code users could alternatively use ISO = 1 and simply provide the parameter values E, G, and ALPHA for Young's modulus, Poisson's ratio, and the isotropic thermal expansion coefficient, respectively. Input parameter values of zero are not required in the namelist formats of the TCCATE code; but null values of some input variables are frequently included in namelists for the sake of editing convenience. Plane strain calculations are executed for NGE0 = 1, and the default value NGE0 = 0 executes plane stress calculations. The discussion from Equation (64) to Equation (94) in the text describes technical distinctions between these options. The parameter INTEG = 4 implements fourth-order quadrature integration formulae in computations of material displacements.

2. Output

The stress code option which is executed by the input data above produces as output (i) a file named OUTPUT which contains stress data tabulations for users, and (ii) a graphics data file named PLTUAT which is to be used with the utility routine GRAFCON for plotting the computed stress data. The OUTPUT file appears below; it first presents a self-explanatory summary of the problem parameters which have been read by the code from the input data file HOPS. This problem control information is followed by tabulated values of temperatures and by a report of the convergence history of the DAVI solution process. This data is followed by tabulations of computed stress potential, stress components ($S_{xx} \equiv \sigma_{xx}$, $S_{xy} \equiv \sigma_{xy}$, and $S_{yy} \equiv \sigma_{yy}$), strain components ($E_{xx} \equiv \epsilon_{xx}$, $E_{xy} \equiv \epsilon_{xy}$, and $E_{yy} \equiv \epsilon_{yy}$), and material displacement components u and v. Finally, the computed average (or designated reference) temperature for the slab and computer execution timings are given.

The entire graphical output for this sample problem appears directly below. This GRAFCON job was executed with the command file CONIN which also appears below. GRAFCON commands are described in Reference 13. The solid lines in the contour plots denote positive values of the dependent variables, and the dashed contour lines denote negative values for dependent variables.

OUTPUT - SAMPLE PROBLEM 1

C O N T R O L I N F O R M A T I O N

Stress calculation (IPROB = 2)

Slab temperatures given as a polynomial (JPROB = 1)

Non-zero polynomial coefficients:

c01 = 4.0000 c02 = -4.0000

Slab width (WIDTH)	=	5.0000
Slab height (HT)	=	1.0000
Slab angle in degrees (ANGLE)	=	90.000
Number of grid columns (NCOL)	=	65
Number of grid rows (NROW)	=	33
Print every (NEACHC) column	=	8
Print every (NEACHR) row	=	4
Reduction factor (REDN)	=	1.00000e-07
Maximum number of iterations (NLOOP)	=	250
Order of boundary extrapolation (JEXTRP)	=	4
Order of displacement integration (INTEG)	=	4
Reference temperature flag (ITREF)	=	1
Reference temperature (ITREF)	=	0.66666

SLAB MATERIAL CONSTANTS

Plane strain calculation (NGEO = 1)
 Input select flag for elastic const (150) - 0

Thermal expansion matrix elt	a11 (ALPH11)	=	6.960000e-06
Thermal expansion matrix elt	a22 (ALPH22)	=	6.960000e-06
Thermal expansion matrix elt	a33 (ALPH33)	=	6.960000e-06
Thermal expansion matrix elt	a12 (ALPH12)	=	0.000000
Compliance matrix element	s11 (S11)	=	3.590000e-13
Compliance matrix element	s12 (S12)	=	-9.000000e-14
Compliance matrix element	s13 (S13)	=	-9.000000e-14
Compliance matrix element	s16 (S16)	=	0.000000
Compliance matrix element	s22 (S22)	=	3.590000e-13
Compliance matrix element	s23 (S23)	=	-9.000000e-14
Compliance matrix element	s26 (S26)	=	0.000000
Compliance matrix element	s33 (S33)	=	3.590000e-13
Compliance matrix element	s36 (S36)	=	0.000000
Compliance matrix element	s66 (S66)	=	8.980000e-13

S L A B T E M P E R A T U R E S

\col	1	9	17	25	33	41	49	57
row\								
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.43750	0.43750	0.43750	0.43750	0.43750	0.43750	0.43750	0.43750
9	0.75000	0.75000	0.75000	0.75000	0.75000	0.75000	0.75000	0.75000
13	0.93750	0.93750	0.93750	0.93750	0.93750	0.93750	0.93750	0.93750
17	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
21	0.93750	0.93750	0.93750	0.93750	0.93750	0.93750	0.93750	0.93750
25	0.75000	0.75000	0.75000	0.75000	0.75000	0.75000	0.75000	0.75000
29	0.43750	0.43750	0.43750	0.43750	0.43750	0.43750	0.43750	0.43750
33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

\col	65
row\	
1	0.00000
5	0.43750
9	0.75000
13	0.93750
17	1.00000
21	0.93750
25	0.75000
29	0.43750
33	0.00000

CONVERGENCE HISTORY

step	delt	tp	change	rel error	residual	norm(u)	max(u)	min(u)
1	4.883e-06	0.042	a., 0	1.000e+00	7.831e-01	4.34442e+02	7.41627e+02	0.
2	3.906e-05	0.144	a., 2	7.173e-01	4.016e-01	1.51831e+03	2.75169e+03	0.
3	7.813e-05	0.611	a., 1/7	1.130e-02	2.950e-01	1.52198e+03	2.73597e+03	0.
4	1.116e-05	2.381	a., 1/17	0.279e-04	2.716e-01	1.52166e+03	2.73637e+03	0.
5	6.565e-07	0.685	a., 1/11	0.769e-04	1.981e-01	1.52165e+03	2.73804e+03	0.
6	5.968e-08	0.366	a., 1/5	1.310e-04	1.109e-01	1.52165e+03	2.73784e+03	0.
7	1.194e-08	0.617	a., 1/7	1.020e-05	3.773e-02	1.52165e+03	2.73782e+03	0.
8	1.705e-09	0.188	a., 2	1.452e-06	1.236e-02	1.52165e+03	2.73782e+03	0.
9	3.410e-09	0.049	a., 0	7.206e-07	2.488e-03	1.52165e+03	2.73782e+03	0.
10	2.728e-08	0.037	a., 0	3.836e-06	1.777e-03	1.52165e+03	2.73780e+03	0.
11	2.183e-07	0.083	a., 4	1.418e-05	0.327e-04	1.52164e+03	2.73774e+03	0.
12	8.731e-07	0.060	a., 4	2.465e-05	3.020e-04	1.52163e+03	2.73767e+03	0.
13	3.492e-06	0.048	a., 8	4.765e-05	1.667e-04	1.52157e+03	2.73762e+03	0.
14	2.794e-05	0.135	a., 2	1.400e-04	7.919e-05	1.52138e+03	2.73747e+03	0.
15	5.588e-05	0.269	a., 2	1.777e-05	3.094e-05	1.52136e+03	2.73741e+03	0.
16	1.118e-04	0.600	a., 1/7	1.049e-06	2.930e-05	1.52136e+03	2.73741e+03	0.
17	1.596e-05	1.502	a., 1/17	7.740e-08	2.812e-05	1.52136e+03	2.73741e+03	0.

***** CONVERGENCE ACHIEVED *****

Total number of steps = 17
Number of successful steps = 17
Number of rejected steps = 0
CPU time for solution 0.168 (sec)
CPU time per step 0.010 (sec)
CPU time per grid point 0.008 (sec)

CALCULATED SLAB STRESS POTENTIAL

\col	1	9	17	25	33	41	49	57
row\								
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	90208.	0.10344e+06	0.10325e+06	0.10318e+06	0.10325e+06	0.10344e+06	90208.
9	0.00000	0.26047e+06	0.30373e+06	0.30344e+06	0.30321e+06	0.30344e+06	0.30373e+06	0.26047e+06
13	0.00000	0.40261e+06	0.47431e+06	0.47414e+06	0.47377e+06	0.47414e+06	0.47431e+06	0.40261e+06
17	0.00000	0.45642e+06	0.53955e+06	0.53947e+06	0.53905e+06	0.53947e+06	0.53955e+06	0.45642e+06
21	0.00000	0.40261e+06	0.47431e+06	0.47414e+06	0.47377e+06	0.47414e+06	0.47431e+06	0.40261e+06
25	0.00000	0.26047e+06	0.30373e+06	0.30344e+06	0.30321e+06	0.30344e+06	0.30373e+06	0.26047e+06
29	0.00000	90208.	0.10344e+06	0.10325e+06	0.10318e+06	0.10325e+06	0.10344e+06	90208.
33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

\col	65
row\	
1	0.00000
5	0.00000
9	0.00000
13	0.00000
17	0.00000
21	0.00000
25	0.00000
29	0.00000
33	0.00000

SLAB STRESS COMPONENT SXX

\col	1	9	17	25	33	41	49	57
row\								
1	0.00000	1.54683e+07	1.73287e+07	1.72768e+07	1.72659e+07	1.72768e+07	1.73287e+07	1.54683e+07
5	-1.06137e-09	4.80974e+06	5.92386e+06	5.93501e+06	5.92972e+06	5.93501e+06	5.92386e+06	4.80974e+06
9	-9.50735e-10	-2.05221e+06	-2.17353e+06	-2.15713e+06	-2.15601e+06	-2.15713e+06	-2.17353e+06	-2.05221e+06
13	-4.72646e-10	-5.86829e+06	-7.01044e+06	-7.01339e+06	-7.00771e+06	-7.01339e+06	-7.01044e+06	-5.86829e+06
17	2.80450e-22	-7.00988e+06	-8.61843e+06	-8.63230e+06	-8.62581e+06	-8.63230e+06	-8.61843e+06	-7.00988e+06
21	4.72646e-10	-5.86829e+06	-7.01044e+06	-7.01339e+06	-7.00771e+06	-7.01339e+06	-7.01044e+06	-5.86829e+06
25	9.50735e-10	-2.05221e+06	-2.17353e+06	-2.15713e+06	-2.15601e+06	-2.15713e+06	-2.17353e+06	-2.05221e+06
29	1.06137e-09	4.80974e+06	5.92386e+06	5.93501e+06	5.92972e+06	5.93501e+06	5.92386e+06	4.80974e+06
33	0.00000	1.54683e+07	1.73287e+07	1.72768e+07	1.72659e+07	1.72768e+07	1.73287e+07	1.54683e+07

\col	65
row\	
1	0.00000
5	1.06137e-09
9	9.50735e-10
13	4.72646e-10
17	1.46631e-21
21	-4.72646e-10
25	-9.50735e-10
29	-1.06137e-09
33	0.00000

SLAB STRESS COMPONENT S Y Y

\col	1	9	17	25	33	41	49	57
row\								
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	2.56327e+06	-0.28077e+06	-15242.	1058.7	213.95	1058.7	-15242.	-0.28077e+06
9	7.23710e+06	-0.83203e+06	-53599.	2912.4	709.85	2912.4	-53599.	-0.83203e+06
13	1.07026e+07	-1.30200e+06	-92287.	4318.3	1185.7	4318.3	-92287.	-1.30200e+06
17	1.19320e+07	-1.40136e+06	-0.10029e+06	4016.1	1370.1	4016.1	-0.10029e+06	-1.40136e+06
21	1.07026e+07	-1.30200e+06	-92287.	4318.3	1185.7	4318.3	-92287.	-1.30200e+06
25	7.23710e+06	-0.83203e+06	-53599.	2912.4	709.85	2912.4	-53599.	-0.83203e+06
29	2.56327e+06	-0.28077e+06	-15242.	1058.7	213.95	1058.7	-15242.	-0.28077e+06
33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

\col	65
row\	
1	0.00000
5	2.56327e+06
9	7.23710e+06
13	1.07026e+07
17	1.19320e+07
21	1.07026e+07
25	7.23710e+06
29	2.56327e+06
33	0.00000

S L A B S T R E S S C O M P O N E N T S X Y

row\col	1	9	17	25	33	41	49	57
1	0.00000	5159.0	-463.59	-38.757	4.76037e-08	38.757	463.59	-5159.0
5	0.30941e+06	-9.81511e+05	-20376.	4579.5	-4.71274e-06	-4579.5	20376.	9.81511e+05
9	0.27716e+06	-1.22302e+06	-38079.	3362.9	-6.03467e-06	-5362.9	38079.	1.22302e+06
13	0.13779e+06	-0.79973e+06	-29022.	3366.8	-2.86102e-06	-3366.8	29022.	0.79973e+06
17	-9.19085e-08	-3.62112e-06	9.90898e-06	-2.16167e-06	-8.90898e-07	-1.30735e-05	1.52656e-06	7.69551e-06
21	0.13779e+06	0.79973e+06	38076.	-3366.8	7.62937e-07	3366.8	-29022.	-0.79733e+06
25	-0.27716e+06	1.22302e+06	38079.	-3362.9	4.13255e-06	5362.9	-38079.	-1.22302e+06
29	-0.30941e+06	9.81511e+05	20376.	-4579.5	7.59761e-03	4579.5	-20376.	9.81511e+05
33	0.00000	-5159.0	463.59	38.757	-1.37091e-07	-38.757	-463.59	5159.0

row\col	65
1	0.00000
5	-0.30941e+06
9	-0.27716e+06
13	-0.13779e+06
17	-4.37697e-07
21	0.13779e+06
25	0.27716e+06
29	0.30941e+06
33	0.00000

SLAB STRAIN COMPONENT E X X

row\col	1	9	17	25	33	41	49	57
1	-5.88323e-06	-5.99104e-07	2.67748e-08	9.34386e-09	5.64890e-09	9.34386e-09	2.67748e-08	-5.99104e-07
5	-2.28339e-06	-3.45888e-07	-1.37183e-10	1.77972e-09	9.45563e-11	1.77972e-09	-1.37183e-10	-3.45888e-07
9	-6.92333e-08	1.28628e-07	1.81696e-10	-6.63171e-10	-3.76138e-11	-6.63171e-10	1.81696e-10	1.28628e-07
13	1.15855e-06	5.29688e-07	9.37738e-09	-2.49113e-09	-3.27167e-10	-2.49113e-09	9.37738e-09	5.29688e-07
17	1.5852e-06	6.83661e-07	1.42420e-08	-3.15298e-09	-3.13248e-10	-3.15298e-09	1.42420e-08	6.83661e-07
21	1.15655e-06	5.29888e-07	9.37738e-09	-2.49113e-09	-3.27167e-10	-2.49113e-09	9.37738e-09	5.29888e-07
25	-9.32333e-08	1.28628e-07	1.81696e-10	-6.63171e-10	-3.76138e-11	-6.63171e-10	1.81696e-10	1.28628e-07
29	-2.28339e-06	-3.45888e-07	-1.37183e-10	1.77972e-09	9.45563e-11	1.77972e-09	-1.37183e-10	-3.45888e-07
33	-5.88323e-06	-5.99104e-07	2.67748e-08	9.34386e-09	5.64890e-09	9.34386e-09	2.67748e-08	-5.99104e-07

row\col	65
1	-5.88323e-06
5	-2.28339e-06
9	-6.92333e-08
13	1.15855e-06
17	1.5852e-06
21	1.15655e-06
25	-9.32333e-08
29	-2.28339e-06
33	-5.88323e-06

SLAB STRAIN COMPONENT EYY

\col	1	9	17	25	33	41	49	57
row\								
1	-5.80323e-06	-7.54439e-06	-7.75379e-06	-7.74796e-06	-7.74672e-06	-7.74796e-06	-7.75379e-06	-7.54439e-06
5	-1.13248e-06	-2.63072e-06	-2.66679e-06	-2.66257e-06	-2.66225e-06	-2.66257e-06	-2.66679e-06	-2.63072e-06
9	3.16023e-06	6.76481e-07	9.52029e-07	9.69196e-07	9.68329e-07	9.69196e-07	9.52029e-07	6.76481e-07
13	5.95832e-06	2.58007e-06	3.11563e-06	3.14846e-06	3.14677e-06	3.14846e-06	3.11563e-06	2.58007e-06
17	6.91599e-06	3.20129e-06	3.83530e-06	3.87491e-06	3.87293e-06	3.87491e-06	3.83530e-06	3.20129e-06
21	5.95832e-06	2.58007e-06	3.11563e-06	3.14846e-06	3.14677e-06	3.14846e-06	3.11563e-06	2.58007e-06
25	3.16023e-06	6.76481e-07	9.52029e-07	9.69196e-07	9.68329e-07	9.69196e-07	9.52029e-07	6.76481e-07
29	-1.13248e-06	-2.63072e-06	-2.66679e-06	-2.66257e-06	-2.66225e-06	-2.66257e-06	-2.66679e-06	-2.63072e-06
33	-5.80323e-06	-7.54439e-06	-7.75379e-06	-7.74796e-06	-7.74672e-06	-7.74796e-06	-7.75379e-06	-7.54439e-06

\col	65
row\	
1	-5.80323e-06
5	-1.13248e-06
9	3.16023e-06
13	5.95832e-06
17	6.91599e-06
21	5.95832e-06
25	3.16023e-06
29	-1.13248e-06
33	-5.80323e-06

SLAB STRAIN COMPONENT EXY

row\col	1	9	17	25	33	41	49	57
1	0.00000	2.31640e-09	-2.08154e-10	-1.74021e-11	2.14100e-20	1.74021e-11	2.08154e-10	-2.31640e-09
5	1.38927e-07	-4.40698e-07	-9.14882e-09	2.05620e-09	-2.11602e-10	-2.05620e-09	9.14882e-09	4.40698e-07
9	1.24446e-07	-5.49137e-07	-1.70976e-08	2.40793e-09	-3.06877e-10	-2.40793e-09	1.70976e-08	5.49137e-07
13	6.18667e-08	-3.59081e-07	-1.33902e-08	1.51170e-09	-1.28460e-10	-1.51170e-09	1.33902e-08	3.59081e-07
17	-4.13037e-20	-1.62602e-10	4.45336e-10	-9.70590e-19	-3.99654e-19	-6.56400e-18	6.85203e-19	3.45529e-10
21	-6.18667e-08	3.59081e-07	1.33902e-08	-1.51170e-09	3.42559e-19	1.51170e-09	-1.33902e-08	-3.59081e-07
25	-1.24446e-07	5.49137e-07	1.70976e-08	-2.40793e-09	1.85553e-10	2.40793e-09	-1.70976e-08	-5.49137e-07
29	-1.38927e-07	4.40698e-07	9.14882e-09	-2.05620e-09	3.41132e-10	2.05620e-09	-9.14882e-09	-4.40698e-07
33	0.00000	-2.31640e-09	2.08154e-10	1.74021e-11	-6.15537e-20	-1.74021e-11	-2.08154e-10	2.31640e-09

row\col	65
1	0.00000
5	-1.38927e-07
9	-1.24446e-07
13	-6.18667e-08
17	-1.96526e-19
21	6.18667e-08
25	1.24446e-07
29	1.38927e-07
33	0.00000

SLAB DISPLACEMENT COMPONENT U

\col	1	9	17	25	33	41	49	57
row\								
1	1.91855e-06	6.15260e-08	-1.57409e-08	-4.15132e-09	-2.05426e-18	4.15132e-09	1.57409e-08	-6.15260e-08
5	8.17084e-07	5.80505e-08	-2.45282e-09	-3.67496e-10	-1.01107e-18	3.67496e-10	2.45282e-09	-5.80505e-08
9	-2.04105e-07	-2.18950e-08	8.92248e-10	1.38285e-10	-4.54690e-19	-1.38285e-10	-8.92248e-10	2.18950e-08
13	-9.08277e-07	-1.01814e-07	1.89214e-09	5.79987e-10	-1.36798e-19	-5.79987e-10	-1.89214e-09	1.01814e-07
17	-1.15780e-06	-1.34159e-07	1.99580e-09	7.51606e-10	0.00000	-7.51606e-10	-1.99580e-09	1.34159e-07
21	-9.08277e-07	-1.01814e-07	1.89214e-09	5.79987e-10	-2.60316e-19	-5.79987e-10	-1.89214e-09	1.01814e-07
25	-2.04105e-07	-2.18950e-08	8.92248e-10	1.38285e-10	-4.66722e-19	-1.38285e-10	-8.92248e-10	2.18950e-08
29	8.17084e-07	5.80505e-08	-2.45282e-09	-3.67496e-10	-5.17814e-19	3.67496e-10	2.45282e-09	-5.80505e-08
33	1.91855e-06	6.15260e-08	-1.57409e-08	-4.15132e-09	-5.53263e-19	4.15132e-09	1.57409e-08	-6.15260e-08

\col	65
row\	
1	-1.91855e-06
5	-8.17084e-07
9	2.04105e-07
13	9.08277e-07
17	1.15780e-06
21	9.08277e-07
25	2.04105e-07
29	-8.17084e-07
33	-1.91855e-06

SLAB DISPLACEMENT COMPONENT V

\col	1	9	17	25	33	41	49	57
row\								
1	-1.11260e-06	1.32761e-07	9.07525e-09	-4.27836e-10	-9.54655e-11	-4.27836e-10	9.07525e-09	1.32761e-07
5	-1.55123e-06	-4.85084e-07	-6.26806e-07	-6.35873e-07	-6.35436e-07	-6.35873e-07	-6.26806e-07	-4.85084e-07
9	-1.41259e-06	-5.91700e-07	-7.18753e-07	-7.26581e-07	-7.26181e-07	-7.26581e-07	-7.18753e-07	-5.91700e-07
13	-8.24504e-07	-3.74332e-07	-4.49433e-07	-4.54095e-07	-4.53060e-07	-4.54095e-07	-4.49433e-07	-3.74332e-07
17	-4.67277e-17	-4.59472e-18	2.40550e-17	7.02205e-18	0.00000	6.07353e-18	2.19260e-17	8.95266e-17
21	8.24504e-07	3.74332e-07	4.49433e-07	4.54095e-07	4.53060e-07	4.54095e-07	4.49433e-07	3.74332e-07
25	1.41259e-06	5.91700e-07	7.18753e-07	7.26581e-07	7.26181e-07	7.26581e-07	7.18753e-07	5.91700e-07
29	1.55123e-06	4.85084e-07	6.26806e-07	6.35873e-07	6.35436e-07	6.35873e-07	6.26806e-07	4.85084e-07
33	1.11260e-06	-1.32761e-07	-9.07525e-09	4.27836e-10	9.54655e-11	4.27836e-10	-9.07525e-09	-1.32761e-07

\col	65
row\	
1	-1.11260e-06
5	-1.55123e-06
9	-1.41259e-06
13	-8.24504e-07
17	1.30176e-16
21	8.24504e-07
25	1.41259e-06
29	1.55123e-06
33	1.11260e-06

Average slab temperature = 0.66681

T I M I N G S (S E C)

		CPU	I/O	SYS	
		---	---	---	
CODE INITIALIZATION	>>	0.031	0.017	0.004	
POTENTIAL EQUATION SOLUTION	>>	2.367	0.251	0.012	
		1.125	0.137	0.007	Initialization
		0.170	0.000	0.000	Solution
		0.010	0.000	0.000	Printfile
		1.061	0.114	0.004	Plotfile
STRESS/STRAIN/DISPLACEMENT	>>	9.610	2.790	0.114	
	>	3.208	0.401	0.014	Stresses
		0.001	0.000	0.000	calculation
		0.032	0.000	0.000	printfile
		3.174	0.401	0.013	plotfile
	>	3.199	0.415	0.013	Strains
		0.001	0.000	0.000	calculation
		0.032	0.000	0.000	printfile
		3.165	0.415	0.012	plotfile
	>	2.157	1.017	0.004	Displacements
		0.005	0.000	0.000	calculation
		0.022	0.000	0.000	printfile
		2.130	1.017	0.003	plotfile
	>	1.047	0.070	0.003	Displaced grid
TOTAL TECATE TIME		15.206	12.019	3.057	0.130

FILE CONIN FOR EXECUTING GRAFCON

```

rjet 72
box z46 samp21
mslj 1 65 64 1 33 32
meshon
grtt 2
grtb 2
grtl 2
grtr 2
style ct dotneg
tmds 143
file p:tdat
vp .1 .8 .1 .8
tx ct 118
tx tb 118
title
TEMPERATURE
ctmd 1
frame
job 2
title
STRESS POTENTIAL
ctmd 1
frame
job 3
title
STRESS COMPONENT Sxx
ctmd 1
frame
job 4
title
STRESS COMPONENT Syy
ctmd 1
frame
job 5
title
STRESS COMPONENT Sxy
ctmd 1
frame
job 6
title
STRAIN COMPONENT Exx
ctmd 1
frame
job 7
title
STRAIN COMPONENT Eyy
ctmd 1
frame
job 8
title

```

STRAIN COMPONENT Exy
ctmd 1
frame
job 9
title
DISPLACEMENT COMPONENT U
ctmd 1
frame
job 10
title
DISPLACEMENT COMPONENT V
ctmd 1
frame
job 11
title
DISPLACED GRID
msij 1 65 1 1 33 1
c
tableoff
ctmd 1
meshon
frame

COMPLETE GRAFCON OUTPUT - SAMPLE PROBLEM 1

TEMPERATURE

STRESS POTENTIAL

STRESS COMPONENT S_{xx}

X Axis

STRESS COMPONENT S_{yy}

X Axis

STRESS COMPONENT Sxy

STRAIN COMPONENT ENX

X Axis

X Axis

STRAIN COMPONENT ϵ_{yy}

STRAIN COMPONENT ϵ_{xy}

DISPLACEMENT COMPONENT U

DISPLACEMENT COMPONENT V

X Axis

X Axis

DISPLACED GRID

X Axis

F. SECOND SAMPLE WORK SESSION

We consider as a second sample problem the second example which appeared previously in section IIB. This example was executed as a combined temperature stress computation. The input file HOPS for this problem appears immediately below. All of the variables in this namelist have been described previously. The dopant density in the flashlamp source function is taken to be $RHO = \rho_n = 0.46$ (in units of 10^{20} cm^{-3}) as described in Equations (21)-(23). Film boundary conditions are applied at the top and bottom slab surfaces, and zero-Neumann (adiabatic, or insulating) conditions are applied at the slab end surfaces. The code output tabulations for this combined heat and stress computation appear immediately below, followed by the graphical output for this run.

INPUT FILE HOPS FOR SAMPLE PROBLEM 2.

```

iprob = 0
jprob = 0
$
ncol = 65
nrow = 33
width = 5.
ht = 1.
angle = 90.
neachc = 0
neachr = 4
redn = 1.e-9
nloop = 250
jextrp = 4
cond11 = 1.3e5
cond12 = 0.
cond22 = 1.3e6
neu1 = 2
neu2 = 2
neu3 = 1
neu4 = 1
neumb = 1
ub1 = 0.
ub2 = 0.
ut1 = 0.
utr = 0.
uambb1 = 310.
uambb2 = 300.
uambb3 = 300.
uambb4 = 310.
flmcf1 = 0.
flmcf2 = 0.75e5
flmcf3 = 4.75e5
rho = 0.46
bval = 0.7127
cval = 0.1343
dval = 1.1167
pwrt1 = 2.5e6
pwrt2 = 2.5e6
pwrt3 = 2.5e6
pwrt4 = 2.5e6
iso = 0
alph11 = 6.96e-6
alph22 = 6.96e-6
alph33 = 6.96e-6
alph12 = 0.
s11 = 3.59e-13
s12 = -.9e-13
s13 = -.9e-13
s16 = 0.
s22 = 3.59e-13
s23 = -.9e-13
s26 = 0.
s33 = 3.59e-13
s36 = 0.
s66 = 0.00e-13
ngeo = 1
integ = 4
$

```

C O N T R O L I N F O R M A T I O N

Heat/Stress calculation (IPROB = 0)
 Two absorber flashlamp model (JPROB = 0)
 Dopant density (times 1.e-20) (RHO) = 0.46000
 Source function parameter b (BVAL) = 0.71270
 Source function parameter c (CVAL) = 0.13430
 Source function parameter d (DVAL) = 1.1167
 Power density from top lamp at left (PWRTL) = 2.50000e+06
 Power density from top lamp at right (PWRTR) = 2.50000e+06
 Power density from bottom lamp at left (PWRBL) = 2.50000e+06
 Power density from bottom lamp at right (PWRBR) = 2.50000e+06
 Slab width (WIDTH) = 5.0000
 Slab height (HT) = 1.0000
 Slab angle in degrees (ANGLE) = 90.000
 Number of grid columns (NCOL) = 65
 Number of grid rows (NROW) = 33
 Print every (NEACHC) column = 8
 Print every (NEACHR) row = 4
 Reduction factor (REDN) = 1.00000e-09
 Maximum number of iterations (NLOOP) = 250
 Order of boundary extrapolation (JEXTRP) = 4
 Order of displacement integration (INTEG) = 4
 Reference temperature flag (ITREF) = 0

S L A B M A T E R I A L C O N S T A N T S

Conductivity matrix element k11 (COND11) = 1.30000e+06
Conductivity matrix element k12 (COND12) = 0.00000
Conductivity matrix element k22 (COND22) = 1.30000e+06
Plane strain calculation (NGEO = 1)
Input select flag for elastic coef (ISO) = 0
Thermal expansion matrix elt a11 (ALPH11) = 6.96000e-06
Thermal expansion matrix elt a22 (ALPH22) = 6.96000e-06
Thermal expansion matrix elt a33 (ALPH33) = 6.96000e-06
Thermal expansion matrix elt a12 (ALPH12) = 0.00000
Compliance matrix element s11 (S11) = 3.59000e-13
Compliance matrix element s12 (S12) = -9.00000e-14
Compliance matrix element s13 (S13) = -9.00000e-14
Compliance matrix element s16 (S16) = 0.00000
Compliance matrix element s22 (S22) = 3.59000e-13
Compliance matrix element s23 (S23) = -9.00000e-14
Compliance matrix element s26 (S26) = 0.00000
Compliance matrix element s33 (S33) = 3.59000e-13
Compliance matrix element s36 (S36) = 0.00000
Compliance matrix element s66 (S66) = 8.69000e-13

H E A T T R A N S F E R B O U N D A R Y C O N D I T I O N S

Neuman conditions on left side (NEUML = 2)

Flux value (FLMCFL) = 0.00000

Neuman conditions on right side (NEUMR = 2)

Flux value (FLMCFR) = 0.00000

Natural conditions on top side (NEUMT = 1)

ambient temp at top left corner (UAMBTl) = 300.00

ambient temp at top right corner (UAMBTR) = 310.00

Film coefficient (FLMCFT) = 0.47500e+06

Natural conditions on bottom side (NEUMB = 1)

ambient temp at bottom left corner (UAMBBL) = 310.00

ambient temp at bottom right corner (UAMBBR) = 300.00

Film coefficient (FLMCFB) = 0.47500e+06

CONVERGENCE HISTORY

[illegible][illegible][illegible][illegible][illegible]

change

[illegible][illegible][illegible]

```

***** CONVERGENCE ACHIEVED *****
Total number of steps = 24
Number of successful steps = 24
Number of rejected steps = 0
CPU time for solution = 0.199 (sec)
CPU time per step = 0.008 (sec)
CPU time per grid point = 0.000 (sec)

```


CONVERGENCE HISTORY

min(u)

[illegible][illegible][illegible]

change

```

99992296844411564265236
9871234567890123456789
+10000000000000000000000
200000000000000000000000

```

[illegible]

```

***** CONVERGENCE ACHIEVED *****
Total number of steps = 22
Number of successful steps = 22
Number of rejected steps = 0
CPU time for solution 0.218 (Sec)
CPU time per step 0.010 (Sec)
CPU time per grid point 0.000 (Sec)

```

CALCULATED SLAB STRESS POTENTIAL

[illegible]

SLAB STRAIN COMPONENT EXX

[illegible][illegible]

SLAB STRAIN COMPONENT EXY

[illegible][illegible]

1037

col	1
104	7.06
103	7.06
102	7.06
101	7.06
100	7.06
99	7.06
98	7.06
97	7.06
96	7.06
95	7.06
94	7.06
93	7.06
92	7.06
91	7.06
90	7.06
89	7.06
88	7.06
87	7.06
86	7.06
85	7.06
84	7.06
83	7.06
82	7.06
81	7.06
80	7.06
79	7.06
78	7.06
77	7.06
76	7.06
75	7.06
74	7.06
73	7.06
72	7.06
71	7.06
70	7.06
69	7.06
68	7.06
67	7.06
66	7.06
65	7.06
64	7.06
63	7.06
62	7.06
61	7.06
60	7.06
59	7.06
58	7.06
57	7.06
56	7.06
55	7.06
54	7.06
53	7.06
52	7.06
51	7.06
50	7.06
49	7.06
48	7.06
47	7.06
46	7.06
45	7.06
44	7.06
43	7.06
42	7.06
41	7.06
40	7.06
39	7.06
38	7.06
37	7.06
36	7.06
35	7.06
34	7.06
33	7.06
32	7.06
31	7.06
30	7.06
29	7.06
28	7.06
27	7.06
26	7.06
25	7.06
24	7.06
23	7.06
22	7.06
21	7.06
20	7.06
19	7.06
18	7.06
17	7.06
16	7.06
15	7.06
14	7.06
13	7.06
12	7.06
11	7.06
10	7.06
9	7.06
8	7.06
7	7.06
6	7.06
5	7.06
4	7.06
3	7.06
2	7.06
1	7.06

9
5
6
9
8
7
5
4
4
1

906856
000000
- - - -
4747

17
2
2
5
5
6
8
9
9
:
:
1
1
1
1

666707666
000010000
111111111
444444444

25
00611
0979057
4893438
2212462
432-21234

7
0770777
- - - - -
9999999

33

3-07 3-08 3-09 3-08 3-08

41
128494
463870
1483345
43212123

07-0777-0777-10777

49
3700
3724
4541
4541
8232
9502
1111
1111

06-0067-06
06-0067-06
06-0067-06
06-0067-06
06-0067-06
06-0067-06

57

66666666
00000000
11111111
22222222

col

Year	1953	1954	1955	1956	1957	1958	1959	1960	1961	1962	1963	1964	1965
1953	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1954	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1955	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1956	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1957	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1958	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1959	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1960	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1961	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1962	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1963	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1964	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7
1965	1.2	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7	1.5	1.3	1.7

SLAB DISPLACEMENT COMPONENT V

[illegible]

col	row	65
1	1	2
1	2	4
1	3	5
1	4	5
1	5	5
1	6	5
1	7	5
1	8	5
1	9	5
1	10	5
1	11	5
1	12	5
1	13	5
1	14	5
1	15	5
1	16	5
1	17	5
1	18	5
1	19	5
1	20	5
1	21	5
1	22	5
1	23	5
1	24	5
1	25	5
1	26	5
1	27	5
1	28	5
1	29	5
1	30	5
1	31	5
1	32	5
1	33	5
1	34	5
1	35	5
1	36	5
1	37	5
1	38	5
1	39	5
1	40	5
1	41	5
1	42	5
1	43	5
1	44	5
1	45	5
1	46	5
1	47	5
1	48	5
1	49	5
1	50	5
1	51	5
1	52	5
1	53	5
1	54	5
1	55	5
1	56	5
1	57	5
1	58	5
1	59	5
1	60	5
1	61	5
1	62	5
1	63	5
1	64	5
1	65	5
1	66	5
1	67	5
1	68	5
1	69	5
1	70	5
1	71	5
1	72	5
1	73	5
1	74	5
1	75	5
1	76	5
1	77	5
1	78	5
1	79	5
1	80	5
1	81	5
1	82	5
1	83	5
1	84	5
1	85	5
1	86	5
1	87	5
1	88	5
1	89	5
1	90	5
1	91	5
1	92	5
1	93	5
1	94	5
1	95	5
1	96	5
1	97	5
1	98	5
1	99	5
1	100	5

Average slab temperature = 305.88

T I M I N G S (S E C)					
		cpu	i/o	sys	
CODE INITIALIZATION	>>	0.048	0.082	0.004	
HEAT TRANSFER SOLUTION	>>	1.850	0.156	0.008	
		0.005	0.000	0.000	Initialization
		0.201	0.000	0.000	Solution
		0.011	0.000	0.000	Printfile
		1.634	0.156	0.007	Plotfile
POTENTIAL EQUATION SOLUTION	>>	1.294	0.065	0.005	
		0.002	0.000	0.000	Initialization
		0.220	0.000	0.000	Solution
		0.010	0.000	0.000	Printfile
		1.062	0.065	0.004	Plotfile
STRESS/STRAIN/DISPLACEMENT	>>	9.593	3.650	0.117	
	>	3.227	0.570	0.015	Stresses
		0.002	0.000	0.000	calculation
		0.032	0.000	0.000	Printfile
		3.194	0.570	0.014	Plotfile
	>	3.163	0.322	0.013	Strains
		0.001	0.000	0.000	calculation
		0.032	0.000	0.000	Printfile
		3.130	0.322	0.013	Plotfile
	>	2.156	2.660	0.086	Displacements
		0.005	0.000	0.000	calculation
		0.022	0.000	0.000	Printfile
		2.130	2.660	0.085	Plotfile
	>	1.046	0.098	0.003	Displaced grid
TOTAL TECATE TIME	16.884	12.798	3.952	0.134	

TEMPERATURE

STRESS POTENTIAL

STRESS COMPONENT σ_{xx}

X Axis

STRESS COMPONENT σ_{yy}

X Axis

STRESS COMPONENT SXX

X Axis

a: -2.50e+05
b: -2.00e+05
c: -1.50e+05
d: -1.00e+05
e: -5.00e+04
f: 0
g: 5.00e+04
h: 1.00e+05
i: 1.50e+05
j: 2.00e+05
k: 2.50e+05

STRAIN COMPONENT EXX

X Axis

a: -7.00e-06
b: -6.00e-06
c: -5.00e-06
d: -4.00e-06
e: -3.00e-06
f: -2.00e-06
g: -1.00e-06
h: 0
i: 1.00e-06
j: 2.00e-06
k: 3.00e-06
l: 4.00e-06
m: 5.00e-06
n: 6.00e-06

STRAIN COMPONENT E_{yy}

STRAIN COMPONENT E_{xy}

DISPLACEMENT COMPONENT U

DISPLACEMENT COMPONENT V

DISPLACED GRID

X Axis

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APPENDICES

Appendix 1

Finite Difference Solutions of Thermoelasticity in Anisotropic Crystals.

An Application of the Dynamic ADI Method

0. Introduction.

The present investigation considers thermoelastic effects which may influence optical propagation in solid laser media with relatively small material deformations. A typical problem can be sketched by noting that relatively low thermal conductivities of doped laser glasses permit thermal peaks to build up within the glass when flashlamp radiation is absorbed. Such thermal peaks can in turn generate thermal stresses which approach tensile yield strengths at only modest average power levels. This type of thermal effect has, in fact, been one limiting factor in the attainment of high average power outputs for glass lasers [1]. Alternatively, various candidate crystals for high average power lasers are known to have thermal conductivities which exceed those of glass by wide margins. But anisotropic crystalline media are subject to such optical propagation effects as stress-induced birefringence which may be a significant determinate of laser performance - even when material deformations are small.

The computational physics research which is reported in this article was undertaken in order to analyze thermally induced stresses for crystal slabs with essentially arbitrary symmetry properties and spatial orientations in practical thermal environments. While these computations are to be carried out presently in two spatial dimensions, it is necessary to retain to the greatest possible extent the actual 3-D symmetry characteristics of the crystals under study. For this, it is necessary to solve accurately the heat equation and Hooke's Law in their general forms which account rigorously for the tensor characteristics of thermal conductivity, thermal expansion, and elastic stiffness properties. Major emphasis is placed upon computing the full material stress tensor with high fidelity. These specific problem requirements have thus prompted new applications of Eulerian discretizations and of a Dynamic Alternating Directions Implicit (DADI) method to fourth-order PDE's of general form for stress potentials in anisotropic media.

This article is organized as follows: section 1 formulates steady-state heat flow computations for anisotropic media in 2-D. Section 2 reviews briefly ADI and DADI theory and their applications for the heat and stress potential equations. Section 3 develops the stress potential PDE's and summarizes essential definitions and compact vector notations for solving stresses, strains, and material displacements; this includes considerations of potential energy concepts which bear upon the positive definiteness of the elastic stiffness matrix and compatibility with the balance of force equations which underly the basic stress potential formulation. Numerically convenient transformations of the PDE's and resultant boundary condition simplifications are introduced. Reductions to the special case of pure plane strain in isotropic media are illustrated. Section 4 presents the discretization scheme which has been developed for the stress potential equations and analyzes the local truncation error properties of the discretization scheme. Section 5 describes numerical approximations which are used in explicit evaluations of material stresses and strains from the computed stress potentials. Section 6 describes closed form calculations of material displacements, which are useful to test the orders of accuracy attained in the numerical calculations. Section 7 presents results of test examples.

1. Heat Flow in Anisotropic Media.

We may typically compute thermally induced stresses, strains, and material displacements on a cross-sectional cut Ω of a laser crystal slab in which the long axial direction of the slab is taken to be practically infinite in the third z -direction which is perpendicular to Ω . Thus, the problems considered in this work are defined on a two-dimensional domain Ω in the x - y plane in the shape of a parallelogram of width a , height b , inner angle α , $0 < \alpha < \pi$, as depicted in Figure 1.1. Such modeling in two independent variables frequently retains the physical rigor of the original three-dimensional theory. For example, when body forces and the temperature distribution in a slab are independent of z , the original 3-D problem can be reduced to the present 2-D problem on the domain Ω . It will be seen that both purely planar and generalised material deformations (in 3-D) can be computed on the domain Ω . (For example, Sample Problem 2 in Section 7 considers trigonal crystals of Al_2O_3 which admit both purely planar and non-planar displacements, according to the crystal orientations which may be considered in practical applications.)

Figure 1.1a
3-D slab which is infinite
in the z -direction

Figure 1.1b
A cross-sectional cut Ω
perpendicular to the z -axis

With these introductory remarks in mind, we develop here the method of reduction and numerical solution of the heat equation by the DADI method (which is described briefly in the next section). Subsequent treatment of thermoelastic stress equations will be conceptually identical to the methods presented here for the heat equation.

The generalised time-dependent heat equation in the crystal slab can be written as

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (K \cdot \nabla T) + Q, \quad (1.1)$$

where

$T \equiv$ temperature (degrees)

$\rho \equiv$ mass density (mass/volume)

$c \equiv$ heat capacity (energy/mass-degree)

$K \equiv$ symmetric thermal conductivity tensor (power/length-degree)

$Q \equiv$ rate of internal heat generation (power/volume)

In the general 3-D problem, the elements of the tensor K are k_{ij} , $1 \leq i, j \leq 3$, and can be written in a matrix form as

$$K = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ k_{12} & k_{22} & k_{23} \\ k_{13} & k_{23} & k_{33} \end{pmatrix}. \quad (1.2)$$

We denote by $\tilde{K}$ the following two-by-two sub-matrix of K

$$\tilde{K} = \begin{pmatrix} k_{11} & k_{12} \\ k_{12} & k_{22} \end{pmatrix}. \quad (1.3)$$

The differential operator ∇ stands as usual for the vector

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right),$$

though later on the same symbol will be used to denote the reduced vector $(\partial/\partial x, \partial/\partial y)$. This should be easily recognised by the context. The product $K \cdot \nabla T$ is the so-called heat flux and is interpreted as the vector

$$K \cdot \nabla T = \begin{pmatrix} k_{11}T_x + k_{12}T_y + k_{13}T_z \\ k_{12}T_x + k_{22}T_y + k_{23}T_z \\ k_{13}T_x + k_{23}T_y + k_{33}T_z \end{pmatrix}.$$

Notice that the heat flux vector in a truly anisotropic medium will not be normal to the isotherms $T = \text{constant}$ as it would be the case if the medium were isotropic. Also notice that it is presently assumed that ρ , c , and the components of the tensor K are all constants, though this assumption can be relaxed to allow these quantities to be functions of the spatial coordinates and even of the temperature T , thereby yielding a nonlinear PDE (See [2]).

Typically, a time-dependent Q looks like a pulse of small time duration. However, if the source Q and the boundary conditions are independent of the time variable, the steady state temperature exists in general and satisfies

$$\nabla \cdot (K \cdot \nabla T) = -Q. \quad (1.4)$$

By restricting ourselves to the two dimensional problem for which the z -dependence is discarded, equation (1.4) on the domain Ω becomes

$$\nabla \cdot (\tilde{K} \cdot \nabla T) \equiv k_{11} \frac{\partial^2 T}{\partial x^2} + 2k_{12} \frac{\partial^2 T}{\partial x \partial y} + k_{22} \frac{\partial^2 T}{\partial y^2} = -Q. \quad (1.5)$$

It is to be emphasized that this study is concerned with finding the solution of equation (1.5), not the time dependent equation (1.1). The temperature T is required to satisfy the following types of boundary conditions on $\partial\Omega$:

- (i) Dirichlet condition: T is a given function on some subset $\partial\Omega_1$ of $\partial\Omega$,
- (ii) Natural Neumann condition: $(\bar{K} \cdot \nabla T) \cdot \nu = -\mu$ on some subset $\partial\Omega_2$ of $\partial\Omega$, where ν is the outward unit normal to $\partial\Omega_2$, and μ is a non-negative function,
- (iii) Film condition: $(\bar{K} \cdot \nabla T) \cdot \nu = -\lambda(T - T_0)$ on $\partial\Omega_3 (= \partial\Omega - \partial\Omega_1 - \partial\Omega_2)$ where T_0 is the "coolant" or "ambient" temperature and the film coefficient λ assumes only positive values.

Notice that in order to obtain a unique solution, the subset $\partial\Omega_2$ must be a proper subset of $\partial\Omega$. It is assumed also that the matrix form (1.2) of the tensor K is positive definite, and therefore the inequality $k_{11}k_{22} > k_{12}^2$ is true; this in turn classifies (1.5) as being an elliptic PDE, thereby making it well-suited for solution by the ADI method.

Transformation of the x - y Plane

One can conveniently map the x - y plane onto the ξ - η plane in such a way that the parallelogram Ω is mapped onto the unit square Γ according to the transformations

$$\begin{aligned}\xi &= (x - y \cot \alpha)/a, \\ \eta &= y/b.\end{aligned}\tag{1.6}$$

Equation (1.5) in the ξ - η plane becomes

$$\kappa_{20} \frac{\partial^2 T}{\partial \xi^2} + 2\kappa_{11} \frac{\partial^2 T}{\partial \xi \partial \eta} + \kappa_{02} \frac{\partial^2 T}{\partial \eta^2} = -Q,\tag{1.7}$$

where

$$\begin{aligned}\kappa_{20} &= \frac{1}{a^2} (k_{11} - 2 \cot \alpha k_{12} + \cot^2 \alpha k_{22}), \\ \kappa_{11} &= \frac{1}{ab} (k_{12} - \cot \alpha k_{22}), \\ \kappa_{02} &= \frac{1}{b^2} k_{22}.\end{aligned}\tag{1.8}$$

By letting κ denote the matrix

$$\kappa = \begin{pmatrix} \kappa_{20} & \kappa_{11} \\ \kappa_{11} & \kappa_{02} \end{pmatrix},\tag{1.9}$$

equation (1.7) can then be written in the divergence form

$$\nabla \cdot (\kappa \cdot \nabla T) = -Q.\tag{1.10}$$

The new coefficients κ_{ij} are indexed so that κ_{ij} is the coefficient of $\partial^{i+j}T/\partial \xi^i \partial \eta^j$. We note that, on the domain Ω , T and Q are functions of x and y , whereas on the unit square Γ and Q become functions of ξ and η through the use of the inverse transformation of (1.6); namely,

$$\begin{aligned}x &= a\xi + b \cot \alpha \eta \\ y &= b\eta\end{aligned}\tag{1.11}$$

One may then write

$$T = T(x, y) = T(x(\xi, \eta), y(\xi, \eta)) = T'(\xi, \eta),$$

$$Q = Q(x, y) = Q(x(\xi, \eta), y(\xi, \eta)) = Q'(\xi, \eta).$$

Since we will be working mostly on the unit square, the primes above can be dropped henceforth for convenience. A similar convention will be used in the stress analysis as well.

As for the boundary conditions of type (ii) and (iii), it can be shown that the directional derivative $(\hat{K} \cdot \nabla T) \cdot \nu$ transforms to $a \sin \alpha (\kappa \cdot \nabla' T) \cdot n$ on the left and right boundaries of Ω , and to $b(\kappa \cdot \nabla' T) \cdot n$ on the top and bottom boundaries, where n denotes the outward unit normal to $\partial\Gamma$, and where $\nabla' = (\partial/\partial\xi, \partial/\partial\eta)$. For the purpose of later reference, the boundary condition of type (iii) becomes (after dropping the prime on ∇').

$$(\kappa \cdot \nabla T) \cdot n = \begin{cases} -\lambda/(a \sin \alpha)(T - T_0) & \text{on } \{\text{left and right sides of } \partial\Gamma\} \cap \partial\Gamma_3 \\ -\frac{\lambda}{b}(T - T_0) & \text{on } \{\text{top and bottom sides of } \partial\Gamma\} \cap \partial\Gamma_3, \end{cases} \quad (1.12)$$

where $\partial\Gamma_3$ is the image of $\partial\Omega_3$ under the map given by (1.6).

Discretisation of the Heat Equation

The continuous heat equation, (1.7) is approximated by first placing a rectangular grid on the unit square and then deriving difference equations at each grid point. We choose a grid which consists of m columns and n rows with uniform mesh spacing $h = 1/(m-1)$ along the ξ -direction and uniform mesh spacing $k = 1/(n-1)$ along the η -direction. As usual, a grid point P or "node" at the intersection of the i^{th} column and the j^{th} row is denoted by $P(i, j)$. An interior node is a node which has four neighboring rectangles or "cells" which lie completely inside the unit square. A boundary node which is not a corner node has only two neighboring cells and a corner node has only one neighboring cell. Auxilliary cells are defined by joining the centers of neighboring cells horizontally and vertically as depicted in Figure 1.2. Any interior node, therefore, is the center of one auxilliary cell; half auxilliary cells are formed at boundary nodes which are not corner nodes, and quarter auxilliary cells are formed at corner nodes.

There are two different ways by which one derives difference equations at nodal points: (i) discretizing each term of equation (1.7) through the use of Taylor expansion, or (ii) integrating both sides of (1.10) on auxilliary cells (including half cells and quarter cells) by use of the divergence theorem and approximating those integrands on the left side which involve first partial derivatives by central difference formulae. The latter approach is preferable, especially at boundary nodes.

Figure 1.2 Neighboring grid cells and auxiliary cells at (a) an interior node $P(i, j)$, and (b) a left boundary node $P(1, j)$. The solid and dotted lines denote grid and auxiliary cell boundaries, respectively.

For an interior node $P(i, j)$, one can approximate the source Q on auxiliary cells by the constant value that Q takes at the center; these two approaches are then identical. The Taylor expansions of $T_{\xi\xi}$, $T_{\xi\eta}$, and $T_{\eta\eta}$ that are used in deriving the difference scheme at an interior node $P(i, j)$, along with the leading truncation error terms are listed below:

$$\begin{aligned} \frac{\partial^2 T}{\partial x^2}(i, j) &= \frac{1}{h^2} (T(i+1, j) - 2T(i, j) + T(i-1, j)) - \frac{h^2}{12} T^{(4,0)} + O(h^4), \\ \frac{\partial^2 T}{\partial y^2}(i, j) &= \frac{1}{k^2} (T(i, j+1) - 2T(i, j) + T(i, j-1)) - \frac{k^2}{12} T^{(0,4)} + O(k^4), \\ \frac{\partial^2 T}{\partial x \partial y}(i, j) &= \frac{1}{4hk} ((T(i+1, j+1) - T(i+1, j-1)) - (T(i-1, j+1) - T(i-1, j-1))) \\ &\quad - \frac{1}{6} (h^2 T^{(3,1)} + k^2 T^{(1,3)}) + O(h^4 + k^4), \end{aligned} \quad (1.13)$$

where $T^{r,s}$ denotes $\partial^{r+s} T / \partial \xi^r \partial \eta^s$ evaluated at node (i, j) . If U denotes the approximate discrete solution to the heat equation, then U is required to satisfy at an interior node the equation

$$\begin{aligned} &\frac{\kappa_{20}}{h^2} (U(i+1, j) - 2U(i, j) + U(i-1, j)) + \frac{\kappa_{02}}{k^2} (U(i, j+1) - 2U(i, j) + U(i, j-1)) \\ &+ \frac{2\kappa_{11}}{4hk} (U(i+1, j+1) - U(i+1, j-1) - (U(i-1, j+1) - U(i-1, j-1))) = -Q(i, j). \end{aligned} \quad (1.14)$$

At a vertical boundary node such as $P(1, j)$ (see Figure 1.2) where a boundary condition of the third type exists, the cell method approach gives

$$\iint_D \nabla \cdot (\kappa \cdot \nabla T) d\xi d\eta = - \iint_D Q d\xi d\eta,$$

where D denotes the half cell with boundary $P_1 P_2 P_3 P_4$. Using the divergence theorem it follows that

$$\oint_{P_1 P_2 P_3 P_4} \left(\kappa_{20} T_\xi + \kappa_{11} T_\eta \right) \cdot n ds = - \iint_D Q d\xi d\eta.$$

Observing that the unit normal n takes on the values $(0, -1)$ along $P_1 P_2$, $(1, 0)$ along $P_2 P_3$, $(0, 1)$ along $P_3 P_4$ and $(-1, 0)$ along $P_4 P_1$ and noting that the integrand $(\kappa \cdot \nabla T) \cdot n$ along the boundary side $P_4 P_1$ is, by (1.12), identical to $-(\lambda/a \sin \alpha)(T - T_0)$, it follows that at $P(1, j)$ the difference scheme becomes (after dividing through by the half cell area)

$$\begin{aligned} & \frac{2\kappa_{20}}{h^2} (U(2, j) - U(1, j)) - \frac{2\lambda_l}{a \sin \alpha h} (U(1, j) - T_0) \\ & + \frac{\kappa_{02}}{k^2} (U(1, j+1) - 2U(1, j) + U(1, j-1)) \\ & + \frac{2\kappa_{11}}{hk} (U(2, j+1) - U(2, j-1)) = -Q(1, j). \end{aligned} \quad (1.15)$$

In equation (1.15), λ_l denotes a constant value of the film coefficient on the vertical left boundary. We introduce the analogous notation λ_r , λ_b , and λ_t to correspond to the values of the film coefficient on the right, bottom, and top sides, respectively. In arriving at (1.15), the temperature values at the corner points P_2 and P_3 of the auxiliary half cell were each approximated by the average of the temperature values at the four nearest neighboring grid points. The temperature values at the midpoints P_1 and P_4 were each approximated by the average of the temperature values at the two nearest neighboring points. For the sake of later reference, we list below the resulting difference schemes for boundary points which lie on the remaining sides of the unit square as well as the corner points:

right boundary $P = P(m, j)$

$$\begin{aligned} & \frac{2\kappa_{20}}{h^2} (U(m-1, j) - U(m, j)) - \frac{2\lambda_r}{a \sin \alpha h} (U(m, j) - T_0) \\ & + \frac{\kappa_{02}}{k^2} (U(m, j+1) - 2U(m, j) + U(m, j-1)) \\ & + \frac{2\kappa_{11}}{hk} (U(m-1, j+1) - U(m-1, j-1)) = -Q(m, j), \end{aligned} \quad (1.16a)$$

bottom boundary $P = P(i, 1)$

$$\begin{aligned} & \frac{\kappa_{20}}{h^2} (U(i+1, 1) - 2U(i, 1) + U(i-1, 1)) \\ & + \frac{2\kappa_{02}}{k^2} (U(i, 2) - U(i, 1)) - \frac{2\lambda_b}{bk} (U(i, 1) - T_0) \\ & + \frac{2\kappa_{11}}{hk} (U(i+1, 2) - U(i-1, 2)) = -Q(i, 1), \end{aligned} \quad (1.16b)$$

top boundary $P = P(i, n)$

$$\begin{aligned} & \frac{\kappa_{20}}{h^2} (U(i+1, n) - 2U(i, n) + U(i-1, n)) \\ & + \frac{2\kappa_{02}}{k^2} (U(i, n-1) - U(i, n)) - \frac{2\lambda_t}{bk} (U(i, n) - T_0) \\ & + \frac{2\kappa_{11}}{hk} (U(i+1, n-1) - U(i-1, n-1)) = -Q(i, n), \end{aligned} \quad (1.16c)$$

corner point $(1, 1)$

$$\begin{aligned} & \frac{2\kappa_{20}}{h^2} (U(2, 1) - U(1, 1)) - \frac{2\lambda_l}{a \sin \alpha h} (U(1, 1) - T_0) \\ & + \frac{2\kappa_{02}}{k^2} (U(1, 2) - U(1, 1)) - \frac{2\lambda_b}{bk} (U(1, 1) - T_0) \\ & + \frac{2\kappa_{11}}{hk} (U(2, 2) - U(1, 1)) = -Q(1, 1), \end{aligned} \quad (1.16d)$$

corner point $(m, 1)$

$$\begin{aligned} & \frac{2\kappa_{20}}{h^2} (U(m-1, 1) - U(m, 1)) - \frac{2\lambda_r}{a \sin \alpha h} (U(m, 1) - T_0) \\ & + \frac{2\kappa_{02}}{k^2} (U(m, 2) - U(m, 1)) - \frac{2\lambda_b}{bk} (U(m, 1) - T_0) \\ & + \frac{2\kappa_{11}}{hk} (U(m-1, 2) - U(m, 1)) = -Q(m, 1), \end{aligned} \quad (1.16e)$$

corner point (m, n)

$$\begin{aligned} & \frac{2\kappa_{20}}{h^2} (U(m-1, n) - U(m, n)) - \frac{2\lambda_r}{a \sin \alpha h} (U(m, n) - T_0) \\ & + \frac{2\kappa_{02}}{k^2} (U(m, n-1) - U(m, n)) - \frac{2\lambda_t}{bk} (U(m, n) - T_0) \\ & + \frac{2\kappa_{11}}{hk} (U(m-1, n-1) - U(m, n)) = -Q(m, n), \end{aligned} \quad (1.16f)$$

corner point $(1, n)$

$$\begin{aligned} & \frac{2\kappa_{20}}{h^2} (U(2, n) - U(1, n)) - \frac{2\lambda_l}{a \sin \alpha h} (U(1, n) - T_0) \\ & + \frac{2\kappa_{02}}{k^2} (U(1, n-1) - U(1, n)) - \frac{2\lambda_t}{\delta k} (U(1, n) - T_0) \\ & + \frac{2\kappa_{11}}{hk} (U(2, n-1) - U(1, n)) = -Q(1, n). \end{aligned} \quad (1.16g)$$

It can be readily shown that the difference equation (1.15) approximates the boundary condition (1.12) to within $O(h^2 + k^2)$ truncation error. However, the PDE itself is approximated to within $O(h + k^2/h)$ truncation error. Similar statements hold for equations (1.16).

Using the usual horizontal bottom-to-top ordering of the grid points of Γ , one obtains the discrete elliptic equation

$$LU = F, \quad (1.17)$$

which corresponds to the totality of equations (1.14), (1.15), and (1.16) as P runs over all the grid points with this ordering. In the next section we discuss the solution method which is used to solve equation (1.17).

2. Dynamic ADI Solution Method

Dynamic ADI seeks to accelerate by automated means the convergence of standard ADI which is very powerful in solving elliptic PDE's. Because not only the heat equation but also the higher-order stress potential equations in the present investigation are amenable to numerical solution by ADI type methods, we have invoked the additional power of DADI method. In order to describe the DADI method efficiently we review briefly the general theory.

ADI Method

Consider the problem of finding the solution u of the finite difference or finite element equation

$$Lu = f, \quad (2.1)$$

where L is a linear elliptic operator and f is a given function. Assume that L can be written as the sum

$$L = A + B, \quad (2.2)$$

where A and B are: (i) negative definite, (ii) easily invertible, and (iii) $AB = BA$. In the non-linear case, it is the Frechét derivative of L that should possess these properties.

The Peaceman-Rachford approach [12] for solving (2.1)-(2.2) is applied heuristically as follows: $Lu \equiv (A+B)u = f$ is converted into the evolution equation

$$\begin{aligned} \frac{\partial v}{\partial t} &= Av + Bv - f, \quad t > 0 \\ v &= \text{some initial guess } u^0 \text{ at } t = 0, \end{aligned} \quad (2.3)$$

whose steady state solution, $t = \infty$, is obviously a solution to $(A+B)u = f$. One proceeds to discretize (2.3) in time, solving odd-numbered steps $(n+1)$ implicitly in A and explicitly in B (also termed the x -sweep) according to

$$\frac{u^{n+1} - u^n}{\Delta t} = Au^{n+1} + Bu^n - f. \quad (2.4)$$

Then, reversing the process, even-numbered steps $(n+2)$ are solved explicitly in A and implicitly in B (the y -sweep) according to

$$\frac{u^{n+2} - u^{n+1}}{\Delta t} = Au^{n+1} + Bu^{n+2} - f. \quad (2.5)$$

The true power of the ADI method comes to bear only when one uses variable Δt . One appropriately chooses a short sequence $0 < \Delta t_1 < \dots < \Delta t_r$ and scans through r double sweeps of the ADI process starting with $\Delta t = \Delta t_1$ and ending with $\Delta t = \Delta t_r$, thereby completing one full ADI iteration. Of course one is not trying to find the true transient solution, but rather to reach the steady state as quickly as possible. The ADI strategy attempts to reduce large eigencomponents of the error with the small values of Δt and to dampen small eigencomponents using larger Δt .

The DADI Method

The innovation of DADI as opposed to standard ADI is the development of a strategy which automatically changes the stepsize Δt dynamically. In this way DADI should be able to : (i) keep Δt within regions of fast convergence; (ii) recognize and suppress instabilities (by decreasing Δt) as they start to develop; and (iii) avoid the beleaguering a priori choice of iteration parameters in the standard ADI method.

Convergence Factor CF

If we denote the steady state solution by u and define the n^{th} error by

$$e^n = u - u^n, \quad (2.6)$$

it is readily shown that

$$e^{n+2} = ((1 + \Delta t A)(1 + \Delta t B))^{-1} ((1 - \Delta t A)(1 - \Delta t B)) e^n. \quad (2.7)$$

Assuming that e^n is an eigenvector for A and hence B with eigenvalues $-\lambda$ and $-\mu$ respectively, it follows from (2.7) that the reduction factor R for a single double sweep is given by

$$e^{n+2} = \left(\frac{1 - \lambda \Delta t}{1 + \lambda \Delta t} \right) \left(\frac{1 - \mu \Delta t}{1 + \mu \Delta t} \right) e^n \equiv R(\lambda \Delta t, \mu \Delta t) e^n. \quad (2.8)$$

Starting from step $n+2$ and performing another double sweep one then obtains u^{n+4} and the error $e^{n+4} = u^{n+4} - u$. Hence the convergence factor CF for two double sweeps (in the sense of the l_2 norm) becomes

$$CF = \frac{\|e^{n+4}\|}{\|e^n\|} \equiv R^2(\lambda \Delta t, \mu \Delta t). \quad (2.9)$$

Test Parameter TP

In order to devise a strategy for DADI (and strictly for bookkeeping purposes) we back up to the n^{th} step and perform one giant double sweep with stepsize $2\Delta t$. This double sweep generates the value $\tilde{u}^{n+4}$ and the error $\tilde{e}^{n+4} = \tilde{u}^{n+4} - u$, where it follows from (2.8) that

$$e^{n+4} = R(2\lambda \Delta t, 2\mu \Delta t) e^n. \quad (2.10)$$

The test parameter TP , an estimate of the relative local truncation error, is then defined by

$$TP = \frac{\|u^{n+4} - \tilde{u}^{n+4}\|}{\|u^{n+4} - u^n\|} = \frac{\|e^{n+4} - \tilde{e}^{n+4}\|}{\|e^{n+4} - e^n\|}. \quad (2.11)$$

In terms of the reduction factor R , the test parameter can also be written as

$$TP = \left| \frac{R^2(\lambda \Delta t, \mu \Delta t) - R(2\lambda \Delta t, 2\mu \Delta t)}{R^2(\lambda \Delta t, \mu \Delta t) - 1} \right|. \quad (2.12)$$

DADI strategy is based on the conclusion that it is possible (for all values of λ and μ) to always make CF reasonably small by merely changing Δt so that TP is confined to a certain range. The strategy used here allows Δt to increase rapidly for small values of TP ($\leq .1$), and to decrease more rapidly for the larger values of TP ($\geq .3$); otherwise Δt is allowed to vary gradually ($.1 \leq TP \leq .3$).

A Stable ADI Type Scheme for the Heat Equation

We present here a stable ADI type scheme for the numerical solution of the elliptic heat equation

$$L_2 u \equiv a_{20}u_{xx} + 2a_{11}u_{xy} + a_{02}u_{yy} = f, \quad (2.13)$$

and the elliptic fourth-order biharmonic equation

$$L_4 u \equiv u_{xxxx} + 2u_{xxyy} + u_{yyyy} = f. \quad (2.14)$$

The finite difference approximation to (2.13) can be written as

$$L_2 U \equiv (A_2 + B_2 + C_2)U = F, \quad (2.15)$$

where A_2 , B_2 , and C_2 correspond essentially to the discretization of u_{xx} , u_{yy} , and u_{xy} , respectively. Similarly for the biharmonic equation, we obtain

$$L_4 U \equiv (A_4 + B_4 + C_4)U = F, \quad (2.16)$$

where A_4 , B_4 , and C_4 correspond essentially to the discretization of u_{xxxx} , u_{yyyy} , and u_{xxyy} , respectively.

An ADI type double sweep for solving (2.15) is defined by:

$$\begin{aligned} \frac{U^{n+1} - U^n}{\Delta t} &= A_2 U^{n+1} + B_2 U^n + C_2 U^n - F, \\ \frac{U^{n+2} - U^{n+1}}{\Delta t} &= A_2 U^{n+1} + B_2 U^{n+2} + C_2 U^n - F. \end{aligned} \quad (2.17)$$

Similarly, an ADI type double sweep for (2.16) is defined by

$$\begin{aligned} \frac{U^{n+1} - U^n}{\Delta t} &= -(A_4 U^{n+1} + B_4 U^n + C_4 U^n - F), \\ \frac{U^{n+2} - U^{n+1}}{\Delta t} &= -(A_4 U^{n+1} + B_4 U^{n+2} + C_4 U^n - F). \end{aligned} \quad (2.18)$$

Notice that the minus sign in (2.18) is required because A_4 and B_4 are positive definite.

Before proceeding to demonstrate the stability of (2.17) and (2.18), we note first that stability of the time dependent integration scheme can be analyzed through the use of Fourier analysis as well. One essentially considers the Fourier components $e^{ik_1 x + k_2 y}$; k_1 and k_2 are wave members and

determines what is known as the symbol or amplification factor $\rho(\Delta t, h, k)$ (or amplification matrix for a system of PDE's) [11]. The numerical scheme is stable if ρ satisfies the Von Neumann condition:

$$\rho \leq 1 + O(\Delta t).$$

Claim. The schemes (2.17) and (2.18) are unconditionally stable.

Proof. We will only show that (2.17) is unconditionally stable. The proof for (2.18) is similar. Assume $h = k$ and let $\alpha = \frac{\Delta t}{h^2}$, $\theta_1 = k_1 h$, $x = -2(1 - \cos \theta_1)$, $\theta_2 = k_2 h$, and $y = -2(1 - \cos \theta_2)$. It can be shown that the amplification factor is given by

$$\rho = \frac{(1 + a_{20}x)(1 + a_{02}y) - 4a_{11} \sin \theta_1 \sin \theta_2}{(1 - a_{20}x)(1 - a_{02}y)}. \quad (2.19)$$

Using the fact that $a_{20}x^2 + 2k_{11}x + a_{02}$ is positive for all real x , one can show that $|\rho| < 1$.

3. Derivation for the Stress Potentials PDE's.

A. Background Discussion of Stress Variables, Definitions, and Conventions for Crystal Physics.

We are primarily concerned with computing in practical applications the full stress tensor σ in anisotropic solids. Figure 3.1 represents forces on a small volume element in a stressed body.

Figure 3.1. Schematic representation of the forces on a small volume element in a stressed body

The normal components of stress are denoted by σ_{11} , σ_{22} , and σ_{33} ; and the elements σ_{12} , σ_{21} , σ_{23} , etc., denote the shear components of stress. A positive sign of σ_{11} , σ_{22} , σ_{33} implies a tensile stress; a negative sign implies a compressive stress. Because a universally accepted set of notations and conventions apparently does not exist in thermoelasticity at this time, we present here those definitions and conventions which are useful in our considerations of general anisotropic media, and especially of crystals.

Stress Tensor σ : a symmetric second rank tensor σ_{ij} , $1 \leq i, j \leq 3$. In matrix notation we write

$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}; \quad (3.1)$$

equivalently, σ is written in the familiar notation

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}. \quad (3.2)$$

The notation actually used henceforth is the compact notation

$$\sigma = \begin{pmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{pmatrix}. \quad (3.3)$$

Alternatively σ can be written as a six-component vector which is denoted by σ' . Using the notation of (3.3),

$$\sigma' = (\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5, \sigma_6)^t. \quad (3.4)$$

Strain tensor ϵ : a symmetric second rank tensor ϵ_{ij} , $1 \leq i, j \leq 3$, written in matrix forms similar to those used above for the stress tensor as

$$\epsilon = \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{pmatrix} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \begin{pmatrix} \epsilon_1 & \epsilon_6/2 & \epsilon_5/2 \\ \epsilon_6/2 & \epsilon_2 & \epsilon_4/2 \\ \epsilon_5/2 & \epsilon_4/2 & \epsilon_3 \end{pmatrix}. \quad (3.5)$$

The strain vector is defined by

$$\epsilon' = (\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5, \epsilon_6)^t. \quad (3.6)$$

Thermal Expansion Tensor α :

$$\alpha = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix} = \begin{pmatrix} \alpha_1 & \alpha_6/2 & \alpha_5/2 \\ \alpha_6/2 & \alpha_2 & \alpha_4/2 \\ \alpha_5/2 & \alpha_4/2 & \alpha_3 \end{pmatrix} \quad (3.7)$$

The thermal expansion vector α' is defined by

$$\alpha' = (\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6)^t. \quad (3.8)$$

The rationale for the choice of the factors of $\frac{1}{2}$ appearing in the compact notation will be discussed in Appendix A, which is concerned with the effect of orthogonal coordinate transformations on the symmetric second rank tensors σ , ϵ , and α .

The Displacement Vector : a vector denoted by $\vec{d} = (u, v, w)^t$ which is defined at a point P with position vector $\vec{r} = (x, y, z)^t$ in the undeformed frame of reference x, y, z such that $\vec{d} + \vec{r}$ is the new position vector of P in the deformed state.

The Strain-Displacement Relations :

$$\begin{aligned} \epsilon_1 &= \frac{\partial u}{\partial x} & \epsilon_4 &= \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \\ \epsilon_2 &= \frac{\partial v}{\partial y} & \epsilon_5 &= \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \\ \epsilon_3 &= \frac{\partial w}{\partial z} & \epsilon_6 &= \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \end{aligned} \quad (3.10)$$

Generalized Hooke's Law : For small deformations, the stress-strain relation is given by the linear relation

$$\epsilon' = S\sigma' + \alpha'T, \quad (3.11)$$

where S is the so-called compliance matrix, $S = (s_{ij})$.

In order to provide the logical basis for the thermal stress computations which are considered in later sections, based upon equation (3.11), it is well to recall briefly at this stage some of the basic conventions in crystal physics.

Crystal Physics Conventions.

We follow closely the approach of Nye [3]. Neumann's principle states that each physical constant of a crystal must include every element of symmetry in the point group of the crystal; this principle thus requires compliance of such physical properties as thermal conduction, thermal expansion, elasticity, and stress-optical effects with the symmetry of the crystal. The symmetry conventions used in computations in the present work follow closely the notation and terminology found in International Tables for X-Ray Crystallography [5] and the IRE standards on Piezoelectric Crystals [6]. As indicated in Figure 3.2 below, natural crystal axes

Figure 3.2. Natural crystal axes are defined by sides of a unit cell, Oa , Ob , Oc or simply as the axes a , b , c . Interaxial angles are denoted by α , β , γ .

Oa , Ob , Oc (or simply a , b , c) are parallel to the edges of a unit cell. Theory and computations are developed in terms of orthogonal axes x_1 , x_2 , x_3 which must be related to a , b , c according to arbitrary conventions in order to avert confusion. For example, the x_3 coordinate axis is aligned parallel to the c -axis of a trigonal Al_2O_3 crystal which is considered in a later example. There are also three equivalent secondary crystal axes a_1 , a_2 , and a_3 lying at angles 120° apart in a plane normal to the c -axis of a trigonal Al_2O_3 crystal. In this conventional assignment of axes the x_1 coordinate axis is aligned parallel to any one of the a -axes, as shown in Figure 3.3. The assignment of such conventions thus provides a standard representation for the material property data tensors k_{ij} , α_{ij} , and for elastic compliances S which are used in this work. Of course, if crystals are cut in shapes and orientations which do not coincide with the conventional coordinate axes (x_1, x_2, x_3) , the material property data

tensors must be transformed appropriately to the laboratory frame (x, y, z) of the crystals' shape and orientation. These coordinate transformations are described in Appendix A and their effects will be illustrated in a sample problem which appears later.

Figure 3.3 Conventional coordinate axis orientations for the trigonal crystal Al_2O_3 .

B. Further Analysis

Potential Energy per Unit Volume of Elastic Deformation :

Using the compact vector notation introduced above and dropping the primes, the elastic potential energy per unit volume can be written as

$$V = \frac{1}{2} \sum_i \sigma_i \epsilon_i \quad (3.12)$$

The potential energy is frequently defined [7] in the absence of thermal loading as a function of the strain components ϵ_i , $i = 1, \dots, 6$, such that

$$\sigma_i = \frac{\partial V}{\partial \epsilon_i}, \quad i = 1, \dots, 6. \quad (3.13)$$

It can readily be shown that (3.13) implies (3.12). It also follows from (3.13) that the compliance matrix is symmetric. If one accepts as a plausible fact that the potential energy is positive for any non-zero stress vector, the following claim and proof can be made as an important segment in establishing that the stress potential equations which we derive below are elliptic.

Claim. Any six real numbers can be taken to represent the stress vector at one single point.

Proof. let σ_p be a given stress vector at a point P , whose components $\sigma_1, \dots, \sigma_6$ are chosen arbitrarily. Such a choice of σ_p is possible if there exists a displacement vector $\vec{d} = (u, v, w)^t$ in some

neighborhood of P which gives rise to the given stress vector at P . We let ϵ_p be the strain vector which c corresponds to σ_p , and we assume that the point P is at the origin. With the additional assumption of zero rigid body motion, it can be shown that

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} \epsilon_1 & \epsilon_6/2 & \epsilon_5/2 \\ \epsilon_6/2 & \epsilon_2 & \epsilon_4/2 \\ \epsilon_5/2 & \epsilon_4/2 & \epsilon_3 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + O(r^2). \quad (3.14)$$

Corollary. *The fact that the potential energy V is positive implies that S is positive definite.*

Proof: Indeed, $V = \frac{1}{2} \sigma^t S \sigma$. Thus, provided that σ , at a point, can assume all possible real values, S will be positive definite. The latter assumption is true by the above claim. Using the result of this corollary we show in Appendix B that essential operators L_1 and L_2 (which are to be derived shortly) in the stress potential equations are positive definite.

We are now ready to derive the stress potential PDE's. The general 3-D balance of force equation with zero external body forces is $\nabla \cdot \sigma = 0$. In expanded form

$$\begin{aligned} \frac{\partial \sigma_1}{\partial x} + \frac{\partial \sigma_6}{\partial y} + \frac{\partial \sigma_5}{\partial z} &= 0, \\ \frac{\partial \sigma_6}{\partial x} + \frac{\partial \sigma_2}{\partial y} + \frac{\partial \sigma_4}{\partial z} &= 0, \\ \frac{\partial \sigma_5}{\partial x} + \frac{\partial \sigma_4}{\partial y} + \frac{\partial \sigma_3}{\partial z} &= 0. \end{aligned} \quad (3.15)$$

It is plausible to conclude from the assumptions made in the 2-D problem classification that all stresses are independent of z , and hence by Hooke's Law the strains are also independent of z . The displacement $\vec{d} = (u, v, w)^t$ can also be shown to be independent of z . Geometrically, this implies that the planar domain Ω would in general deform to a non-planar surface. Such deformations will be referred to as generalized plane deformations. The system (3.15) thus reduces to

$$\begin{aligned} \frac{\partial \sigma_1}{\partial x} + \frac{\partial \sigma_6}{\partial y} &= 0, \\ \frac{\partial \sigma_6}{\partial x} + \frac{\partial \sigma_2}{\partial y} &= 0, \\ \frac{\partial \sigma_5}{\partial x} + \frac{\partial \sigma_4}{\partial y} &= 0. \end{aligned} \quad (3.16)$$

Equation (3.16) will frequently be referred to as the reduced set of balance of force equations. The system (3.16) consists of three equations in the five unknowns, $\sigma_1, \sigma_2, \sigma_4, \sigma_5$, and σ_6 . Two more equations are needed in order to determine a unique solution. These extra equations are the so-called compatibility equations. Invoking the fact that the displacement vector d is independent of z in (3.10), it follows that the strains can be defined simply as

$$\begin{aligned} \epsilon_1 &= \frac{\partial u}{\partial x} & \epsilon_2 &= \frac{\partial v}{\partial y} & \epsilon_3 &= 0, \\ \epsilon_4 &= \frac{\partial w}{\partial y} & \epsilon_5 &= \frac{\partial w}{\partial x} & \epsilon_6 &= \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}, \end{aligned} \quad (3.17)$$

and the following compatibility relationships hold:

$$\frac{\partial^2 \epsilon_1}{\partial y^2} - \frac{\partial^2 \epsilon_6}{\partial x \partial y} + \frac{\partial^2 \epsilon_2}{\partial x^2} = 0, \quad (3.18a)$$

$$\frac{\partial \epsilon_4}{\partial x} - \frac{\partial \epsilon_5}{\partial y} = 0. \quad (3.18b)$$

By the use of Hooke's Law in (3.18) one obtains together with (3.16) a system of five PDE's in $\sigma_1, \sigma_2, \sigma_4, \sigma_5, \sigma_6$ of maximum order two. However, for the problem at hand it is more convenient to introduce and solve an alternate formulation for certain potential functions which are defined next.

Potential Solutions: The basic idea is as follows:

1. Stresses are defined as some linear combinations of certain derivatives of potential functions.
2. In terms of these potentials the balance of force equations should be satisfied identically.
3. The number of potentials is equal to the smallest possible number of compatibility equations.
4. These potentials are solutions to the compatibility equations.

In general, these potentials are not unique (see [8]). If more than one set of potentials exist then in addition to the above criteria one attempts to choose those potentials that yield certain desirable characteristics. As a case in point, it can be shown that the potential functions chosen in the following examples are solutions of elliptic systems of PDE's.

Examples:

- i. For the general balance of force equations (3.15), the three potentials ϕ , ψ , and χ are introduced such that

$$\begin{aligned} \sigma_1 &= \frac{\partial^2 \chi}{\partial y^2} + \frac{\partial^2 \psi}{\partial x^2} & \sigma_4 &= -\frac{\partial^2 \phi}{\partial y \partial z} \\ \sigma_2 &= \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \chi}{\partial x^2} & \sigma_5 &= -\frac{\partial^2 \psi}{\partial x \partial z} \\ \sigma_3 &= \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} & \sigma_6 &= -\frac{\partial^2 \chi}{\partial x \partial y} \end{aligned} \quad (3.19)$$

- ii. For the reduced balance of force equations, only two potentials ϕ and ψ are needed. such that

$$\begin{aligned} \sigma_1 &= \frac{\partial^2 \phi}{\partial y^2} & \sigma_2 &= \frac{\partial^2 \phi}{\partial x^2} & \sigma_6 &= -\frac{\partial^2 \phi}{\partial x \partial y} \\ \sigma_3 &= \frac{\partial \psi}{\partial y} & \sigma_4 &= -\frac{\partial \psi}{\partial x} \end{aligned} \quad (3.20)$$

It can readily be shown that (3.19) and (3.20) meet the criteria 1-3.

Finally, using Hookes Law, $\epsilon = S\sigma + \alpha T$, in (3.18) and substituting for σ in terms of the potentials as given in (3.20), one obtains the following system of PDE's for the potentials ϕ and ψ ,

$$L_4 \phi + L_3 \psi = M_2 T, \quad (3.21a)$$

$$L_2 \psi + L_3 \phi = M_1 T, \quad (3.21b)$$

where

$$\begin{aligned}
 L_4 &= s'_{22} \frac{\partial^4}{\partial x^4} - 2s'_{26} \frac{\partial^4}{\partial x^3 \partial y} + (2s'_{12} + s'_{66}) \frac{\partial^4}{\partial x^2 \partial y^2} - 2s'_{16} \frac{\partial^4}{\partial x \partial y^3} + s'_{11} \frac{\partial^4}{\partial y^4}, \\
 L_3 &= -s'_{24} \frac{\partial^3}{\partial x^3} + (s'_{25} + s'_{46}) \frac{\partial^3}{\partial x^2 \partial y} - (s'_{14} + s'_{56}) \frac{\partial^3}{\partial x \partial y^2} + s'_{15} \frac{\partial^3}{\partial y^3}, \\
 L_2 &= s'_{44} \frac{\partial^2}{\partial x^2} - 2s'_{45} \frac{\partial^2}{\partial x \partial y} + s'_{55} \frac{\partial^2}{\partial y^2}, \\
 M_2 &= -\alpha'_2 \frac{\partial^2}{\partial x^2} + \alpha'_6 \frac{\partial^2}{\partial x \partial y} - \alpha'_1 \frac{\partial^2}{\partial y^2}, \\
 M_1 &= \alpha'_4 \frac{\partial}{\partial x} - \alpha'_5 \frac{\partial}{\partial y},
 \end{aligned} \tag{3.22}$$

where s'_{ij} is expressed in terms of s_{ij} by the relation

$$s'_{ij} = s_{ij} - \frac{s_{i3}s_{3j}}{s_{33}}, \tag{3.23}$$

and α'_i is expressed in terms of α_i by the relation

$$\alpha'_i = \alpha_i - \alpha_3 \frac{s_{i3}}{s_{33}}. \tag{3.24}$$

Occasionally we will use the notation

$$\begin{aligned}
 L_4 &= a_{40} \frac{\partial^4}{\partial x^4} + a_{31} \frac{\partial^4}{\partial x^3 \partial y} + a_{22} \frac{\partial^4}{\partial x^2 \partial y^2} + a_{13} \frac{\partial^4}{\partial x \partial y^3} + a_{04} \frac{\partial^4}{\partial y^4}, \\
 L_3 &= a_{30} \frac{\partial^3}{\partial x^3} + a_{21} \frac{\partial^3}{\partial x^2 \partial y} + a_{12} \frac{\partial^3}{\partial x \partial y^2} + a_{03} \frac{\partial^3}{\partial y^3}, \\
 L_2 &= a_{20} \frac{\partial^2}{\partial x^2} + a_{11} \frac{\partial^2}{\partial x \partial y} + a_{02} \frac{\partial^2}{\partial y^2}, \\
 M_2 &= b_{20} \frac{\partial^2}{\partial x^2} + b_{11} \frac{\partial^2}{\partial x \partial y} + b_{02} \frac{\partial^2}{\partial y^2}, \\
 M_1 &= b_{10} \frac{\partial}{\partial x} + b_{01} \frac{\partial}{\partial y}.
 \end{aligned} \tag{3.25}$$

Boundary Conditions.

Let $\nu = (\nu_1, \nu_2, \nu_3)$ be the outward unit normal at a point of the boundary surface boundary; the free surface boundary condition can then be written as

$$\sigma \cdot \nu = 0, \tag{3.26}$$

or in expanded form as

$$\begin{aligned}
 \nu_1 \sigma_1 + \nu_2 \sigma_6 + \nu_3 \sigma_5 &= 0, \\
 \nu_1 \sigma_6 + \nu_2 \sigma_2 + \nu_3 \sigma_4 &= 0, \\
 \nu_1 \sigma_5 + \nu_2 \sigma_4 + \nu_3 \sigma_3 &= 0.
 \end{aligned} \tag{3.27}$$

For the planar domain Ω , $\nu_3 = 0$, and it follows that

$$\begin{aligned}\nu_1\sigma_1 + \nu_2\sigma_6 &= 0, \\ \nu_1\sigma_6 + \nu_2\sigma_2 &= 0, \\ \nu_1\sigma_5 + \nu_2\sigma_4 &= 0.\end{aligned}\tag{3.28}$$

In terms of the potential function given in (3.20), the boundary conditions (3.28) become

$$\begin{aligned}\nu_1 \frac{\partial^2 \phi}{\partial y^2} - \nu_2 \frac{\partial^2 \phi}{\partial x \partial y} &= 0, \\ -\nu_1 \frac{\partial^2 \phi}{\partial x \partial y} + \nu_2 \frac{\partial^2 \phi}{\partial y^2} &= 0, \\ \nu_1 \frac{\partial \phi}{\partial y} - \nu_2 \frac{\partial \phi}{\partial x} &= 0.\end{aligned}\tag{3.29}$$

Transformation of the x - y plane.

We use here exactly the same mapping as was used in our study of the heat equation. Namely, the x - y plane is mapped onto the ξ - η plane in such a way that the parallelogram Ω is mapped onto the unit square Γ according to the co-ordinate transformation

$$\begin{aligned}\xi &= (x - y \cot \alpha)/a, \\ \eta &= y/b,\end{aligned}\tag{3.30}$$

provided that $0 < \alpha < \pi$. It will be shown that the boundary conditions (3.29) are greatly simplified under such a transformation. Observing that

$$\begin{aligned}\frac{\partial}{\partial x} &= \frac{1}{a} \frac{\partial}{\partial \xi}, \\ \frac{\partial}{\partial y} &= -\frac{\cot \alpha}{a} \frac{\partial}{\partial \xi} + \frac{1}{b} \frac{\partial}{\partial \eta},\end{aligned}$$

the PDE's (3.21) transform into

$$L'_4 \phi + L'_3 \psi = M'_2 T, \tag{3.31a}$$

$$L'_2 \psi + L'_3 \phi = M'_1 T, \tag{3.31b}$$

where

$$\begin{aligned}L'_4 &= A_{40} \frac{\partial^4}{\partial \xi^4} + A_{31} \frac{\partial^4}{\partial \xi^3 \partial \eta} + A_{22} \frac{\partial^4}{\partial \xi^2 \partial \eta^2} + A_{13} \frac{\partial^4}{\partial \xi \partial \eta^3} + A_{04} \frac{\partial^4}{\partial \eta^4}, \\ L'_2 &= A_{20} \frac{\partial^2}{\partial \xi^2} + A_{11} \frac{\partial^2}{\partial \xi \partial \eta} + A_{02} \frac{\partial^2}{\partial \eta^2}, \\ L'_3 &= A_{30} \frac{\partial^3}{\partial \xi^3} + A_{21} \frac{\partial^3}{\partial \xi^2 \partial \eta} + A_{12} \frac{\partial^3}{\partial \xi \partial \eta^2} + A_{03} \frac{\partial^3}{\partial \eta^3}, \\ M'_2 &= B_{20} \frac{\partial^2}{\partial \xi^2} + B_{11} \frac{\partial^2}{\partial \xi \partial \eta} + B_{02} \frac{\partial^2}{\partial \eta^2}, \\ M'_1 &= B_{10} \frac{\partial}{\partial \xi} + B_{01} \frac{\partial}{\partial \eta},\end{aligned}\tag{3.32}$$

and where

$$\begin{aligned}
 A_{40} &= (a_{40} - \cot \alpha a_{31} + \cot^2 \alpha a_{22} - \cot^3 \alpha a_{13} + \cot^4 \alpha a_{04})/a^4, \\
 A_{31} &= (a_{31} - 2 \cot \alpha a_{22} + 3 \cot^2 \alpha a_{13} - 4 \cot^3 \alpha a_{04})/(a^3 b), \\
 A_{22} &= (a_{22} - 3 \cot \alpha a_{13} + 6 \cot^2 \alpha a_{04})/(a^2 b^2), \\
 A_{13} &= (a_{13} - 4 \cot \alpha a_{04})/(ab^3), \\
 A_{04} &= a_{04}/b^4, \\
 A_{20} &= (a_{20} - \cot \alpha a_{11} + \cot^2 \alpha a_{02})/a^2, \\
 A_{11} &= (a_{11} - 2 \cot \alpha a_{02})/(ab), \\
 A_{02} &= a_{02}/b^2, \\
 B_{20} &= (b_{20} - \cot \alpha b_{11} + \cot^2 \alpha b_{02})/a^2, \\
 B_{11} &= (b_{11} - 2 \cot \alpha b_{02})/(ab), \\
 B_{02} &= b_{02}/b^2, \\
 A_{30} &= (a_{30} - \cot \alpha a_{21} + \cot^2 \alpha a_{12} - \cot^3 \alpha a_{03})/a^3, \\
 A_{21} &= (a_{21} - 2 \cot \alpha a_{12} + 3 \cot^2 \alpha a_{03})/(a^2 b), \\
 A_{12} &= (a_{12} - 3 \cot \alpha a_{03})/(ab^2), \\
 A_{03} &= a_{03}/(b^3), \\
 B_{10} &= (b_{10} - \cot \alpha b_{01})/a, \\
 B_{01} &= b_{01}/b.
 \end{aligned} \tag{3.33}$$

As for the boundary conditions, the following assertion holds:

Assertion. *To within a rigid body motion, the boundary conditions (3.29) reduce under the transformation (3.30) to*

$$\begin{aligned}
 \phi &= 0, \\
 \frac{\partial \phi}{\partial n} &= 0, \\
 \psi &= 0,
 \end{aligned} \tag{3.34}$$

where n is the outward unit normal to $\partial\Gamma$, the boundary of the unit square.

Proof. Along the top side $y = b$, or $\eta = 1$, $\nu = (0, 1, 0)$ and equations (3.29) reduce to $\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial^2 \phi}{\partial x \partial y} = \frac{\partial \psi}{\partial x} = 0$. Upon integration it follows that, at $y = b$, ϕ is linear in x ; and $\frac{\partial \phi}{\partial y}$ and ψ are constants. Hence, ϕ is linear in ξ , and $\frac{\partial \phi}{\partial \eta}$ and ψ are constant along $\eta = 1$. A similar statement holds true at $\eta = 0$. Along the right boundary, $\nu = (\sin \alpha, -\cos \alpha, 0)$, and by carrying out the ξ - η transformation in (3.29) one obtains

$$\sin \alpha \left(\left(\frac{\cot \alpha}{a} \right)^2 \frac{\partial^2 \phi}{\partial \xi^2} - 2 \frac{\cot \alpha}{ba} \frac{\partial^2 \phi}{\partial \xi \partial \eta} + \left(\frac{1}{b} \right)^2 \frac{\partial^2 \phi}{\partial \eta^2} \right) + \frac{\cos \alpha}{a} \left(-\frac{\cot \alpha}{a} \frac{\partial^2 \phi}{\partial \xi^2} + \frac{1}{b} \frac{\partial^2 \phi}{\partial \xi \partial \eta} \right) = 0,$$

$$\frac{\sin \alpha}{a} \left(-\frac{\cot \alpha}{a} \frac{\partial^2 \phi}{\partial \xi^2} + \frac{1}{b} \frac{\partial^2 \phi}{\partial \xi \partial \eta} \right) + \frac{\cos \alpha}{a^2} \frac{\partial^2 \phi}{\partial \xi^2} = 0,$$

$$\sin \alpha \left(-\frac{\cot \alpha}{a} \frac{\partial \psi}{\partial \xi} + \frac{\partial \psi}{b \partial \eta} \right) + \frac{\cos \alpha}{a} \frac{\partial \psi}{\partial \eta} = 0.$$

Further simplification yields $\frac{\partial^2 \phi}{\partial \xi \partial \eta} \approx \frac{\partial^2 \phi}{\partial \eta^2} \approx \frac{\partial \phi}{\partial \eta} = 0$ which imply that, upon integration along $\xi = 1$, ϕ is a linear function in η and that $\frac{\partial \phi}{\partial \xi}$ and ψ are constant there. A similar statement is true at $\xi = 0$. Invoking the continuity condition of ϕ and ψ at the corner points, it follows that on the boundary, ϕ is an arbitrary linear function which can be taken to be identically equal to 0 (since adding any linear function to ϕ gives rise to the same stress components). Similarly, the continuity of ψ at the corner points requires that ψ can only be a constant along $\partial \Gamma$. Once more from (3.20) we may take $\psi = 0$ on $\partial \Gamma$. It is shown in Appendix B that L_4 and L_2 are elliptic and also that the transformed operators L'_4 and L'_2 remain elliptic. The ADI Method is therefore an attractive solution method for the stress potential equations (3.31).

Pure Plane Strain Equations

These equations are obtained from the generalized plane strain equations (3.17) by assuming that w is identically zero or constant. It follows that both strain components ϵ_4 and ϵ_5 vanish everywhere, and hence the second compatibility relation (3.18b) is satisfied trivially. By criterion 3 of the potential solution requirements, only one potential, ϕ , is needed. It can be shown that equations (3.21) are now replaced by

$$\tilde{L}_4 \phi = \tilde{M}_2 T \quad \text{in } \Gamma, \quad (3.35)$$

subject to the boundary conditions

$$\phi = \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \partial \Gamma, \quad (3.36)$$

where $\tilde{L}_4$ and $\tilde{M}_2$ are of the same form as L_4 and M_2 , respectively. (see equation (3.25))

As an illustration, we consider an isotropic medium with compliance matrix elements

$$s_{11} = s_{22} = s_{33} = \frac{1}{E}, \quad s_{66} = 2(s_{11} - s_{12}) = \frac{2(1 + \nu)}{E},$$

$$s_{12} = s_{21} = s_{13} = s_{31} = s_{23} = s_{32} = \frac{-\nu}{E}, \quad (3.37)$$

where E is Young's modulus and ν is Poisson's ratio. The remaining non-diagonal compliance matrix elements are zeroes. The thermal expansion coefficients are

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha, \quad \alpha_4 = \alpha_5 = \alpha_6 = 0. \quad (3.38)$$

Hooke's Law then takes the simple form

$$\begin{aligned} \epsilon_1 &= s_{11}\sigma_1 + s_{12}\sigma_2 + s_{13}\sigma_3 + \alpha T, \\ \epsilon_2 &= s_{21}\sigma_1 + s_{22}\sigma_2 + s_{23}\sigma_3 + \alpha T, \\ \epsilon_3 &= s_{31}\sigma_1 + s_{32}\sigma_2 + s_{33}\sigma_3 + \alpha T, \\ \epsilon_6 &= s_{66}\sigma_6. \end{aligned} \quad (3.39)$$

Since $\epsilon_3 = 0$ one can eliminate σ_3 in the above system in order to obtain

$$\begin{aligned}\epsilon_1 &= s'_{11}\sigma_1 + s'_{12}\sigma_2 + \alpha'T, \\ \epsilon_2 &= s'_{21}\sigma_1 + s'_{22}\sigma_2 + \alpha'T, \\ \epsilon_6 &= s'_{66}\sigma_6,\end{aligned}\tag{3.40}$$

where, using (3.23), the primed coefficients are given by

$$s'_{11} = s'_{22} = \frac{1 - \nu^2}{E}, \quad s'_{12} = -\frac{\nu(1 + \nu)}{E}, \quad s'_{66} = s_{66}, \quad \alpha' = \alpha(1 + \nu).\tag{3.41}$$

The familiar biharmonic equation in ϕ is obtained [8] either by direct substitution of (3.40) into equation (3.21a) (taking $\psi \equiv 0$) or alternatively by the use of (3.18a) and (3.20); the resultant biharmonic equation is

$$\frac{1 - \nu^2}{E} \left(\frac{\partial^4 \phi}{\partial x^4} + 2 \frac{\partial^4 \phi}{\partial x^2 \partial y^2} + \frac{\partial^4 \phi}{\partial y^4} \right) = -\alpha(1 + \nu) \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right).\tag{3.42}$$

4. **Discretisation of the Potential Equations.** The finite difference approximation of equations (3.31) is considered here. We work with the same grid which is used in the approximation of the heat equation in section 1. Recall that the grid considered there consisted of m columns and n rows with uniform mesh spacings $\Delta\xi = h = 1/(m-1)$ and $\Delta\eta = k = 1/(n-1)$ and that the solution at the gridpoint, or "node", (i, j) is denoted by $\phi(i, j)$. It is useful in the following discussion and in subsequent stress calculations to distinguish among three sets of gridpoints: S_0 is the set of all boundary points; S_1 is the set of all interior nodes having at least one neighbor on the boundary (a neighborhood is the usual 9-point stencil); and S_2 is the set of all interior nodes whose neighbors are also interior nodes.

For a point $P(i, j)$ in S_2 , it is a straight-forward matter to develop and verify the second-order-accurate difference approximations given below for all partial derivatives of ϕ and ψ of order three and four. The first- and second-order partial derivatives are approximated by second-order-accurate difference formulae in equation (2.13). For the mixed derivatives it is simplest to write the differencing formulae in terms of five-by-five stencils centered at (i, j) . In these stencils, "." stands for zero weight, and ϕ^{r+s} denotes $\partial^{r+s}\phi/\partial\xi^r\partial\eta^s$ evaluated at node (i, j) .

$$\frac{\partial^3 \phi}{\partial \xi^3}(i, j) = \frac{1}{2h^3} (\phi(i+2, j) - 2\phi(i+1, j) + 2\phi(i-1, j) - \phi(i-2, j)) - \frac{h^2}{4} \phi^{4,0} + O(h^4) \quad (4.1)$$

$$\frac{\partial^3 \phi}{\partial \eta^3}(i, j) = \frac{1}{2k^3} (\phi(i, j+2) - 2\phi(i, j+1) + 2\phi(i, j-1) - \phi(i, j-2)) - \frac{k^2}{4} \phi^{0,4} + O(k^4) \quad (4.2)$$

$$\frac{\partial^3 \phi}{\partial \xi^2 \partial \eta}(i, j) = \frac{1}{2h^2 k} \begin{bmatrix} . & . & . & . & . \\ . & 1 & -2 & 1 & . \\ . & . & . & . & . \\ . & -1 & 2 & -1 & . \\ . & . & . & . & . \end{bmatrix} \phi(i, j) - \frac{h^2}{12} \phi^{4,1} - \frac{k^2}{6} \phi^{2,3} + O(h^4 + k^4) \quad (4.3)$$

$$\frac{\partial^3 \phi}{\partial \xi \partial \eta^2}(i, j) = \frac{1}{2h k^2} \begin{bmatrix} . & . & . & . & . \\ . & -1 & . & 1 & . \\ . & 2 & . & -2 & . \\ . & -1 & . & 1 & . \\ . & . & . & . & . \end{bmatrix} \phi(i, j) - \frac{h^2}{6} \phi^{3,2} - \frac{k^2}{12} \phi^{1,4} + O(h^4 + k^4) \quad (4.4)$$

$$\frac{\partial^4 \phi}{\partial \xi^4}(i, j) = \frac{1}{h^4} (\phi(i-2, j) - 4\phi(i-1, j) + 6\phi(i, j) - 4\phi(i+1, j) + \phi(i+2, j)) - \frac{h^2}{6} \phi^{6,0} + O(h^4) \quad (4.5)$$

$$\frac{\partial^4 \phi}{\partial \eta^4}(i, j) = \frac{1}{k^4} (\phi(i, j-2) - 4\phi(i, j-1) + 6\phi(i, j) - 4\phi(i, j+1) + \phi(i, j+2)) - \frac{k^2}{6} \phi^{0,0} + O(k^4) \quad (4.6)$$

$$\frac{\partial^4 \phi}{\partial \xi^3 \partial \eta}(i, j) = \frac{1}{4h^3 k} \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & 2 & \cdot & -2 & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & -2 & \cdot & 2 & -1 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \phi(i, j) - \frac{h^2}{4} \phi^{3,1} - \frac{k^2}{6} \phi^{3,3} + O(h^4 + k^4) \quad (4.7)$$

$$\frac{\partial^4 \phi}{\partial \xi^2 \partial \eta^2}(i, j) = \frac{1}{h^2 k^2} \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & -2 & 1 & \cdot \\ \cdot & -2 & 4 & -2 & \cdot \\ \cdot & 1 & -2 & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \phi(i, j) - \frac{1}{12} (h^2 \phi^{4,2} + k^2 \phi^{2,4}) + O(h^4 + k^4) \quad (4.8)$$

$$\frac{\partial^4 \phi}{\partial \xi \partial \eta^3}(i, j) = \frac{1}{4h k^3} \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & 1 & \cdot \\ \cdot & 2 & \cdot & -2 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -2 & \cdot & 2 & \cdot \\ \cdot & 1 & \cdot & -1 & \cdot \end{bmatrix} \phi(i, j) - \frac{k^2}{4} \phi^{1,3} - \frac{h^2}{6} \phi^{3,3} + O(h^4 + k^4) \quad (4.9)$$

We consider next the difference approximations for points belonging to the set S_1 . Essentially the same difference formulae (4.1)–(4.9) are used here, except that one further approximates the value of ϕ (note that ψ does require such an approximation) at points lying outside the logical grid. Such approximations can be obtained by assuming that the solution behaves in a neighborhood of P as a polynomial of some degree p . For example, let the logical coordinate of point P be $(2, j)$ and let us denote the value of ϕ at $(0, j)$, $(1, j)$, $(2, j)$, $(3, j)$, $(4, j)$, and $(5, j)$ by ϕ_0 , ϕ_1 , ϕ_2 , ϕ_3 , ϕ_4 , and ϕ_5 , respectively, and $\frac{\partial \phi}{\partial \xi}$ by ϕ'_1 . The following approximate formulae can then be verified:

Quadratic approximation, $p = 2$,

$$\phi_0 = \phi_1 - 2h\phi'_1 + O(h^3). \quad (4.10)$$

Cubic approximation, $p = 3$,

$$\phi_0 = -\frac{3}{2}\phi_1 + 3\phi_2 - \frac{1}{2}\phi_3 - 3h\phi'_1 + O(h^4). \quad (4.11)$$

Quartic approximation, $p = 4$,

$$\phi_0 = -\frac{10}{3}\phi_1 + 6\phi_2 - 2\phi_3 + \frac{1}{3}\phi_4 - 4h\phi'_1 + O(h^5). \quad (4.12)$$

Quintic approximation, $p = 5$,

$$\phi_0 = -\frac{65}{12}\phi_1 + 10\phi_2 - 5\phi_3 + \frac{5}{3}\phi_4 - \frac{1}{4}\phi_5 - 5h\phi'_1 + O(h^6). \quad (4.13)$$

If one uses the quartic approximation, the discretization of, say, $\frac{\partial^4 \phi}{\partial \xi^4}$ at the point $P(2, j)$ is

$$\frac{\partial^4 \phi}{\partial \xi^4}(2, j) = \frac{1}{h^4}(\phi_0 - 4\phi_1 + 6\phi_2 - 4\phi_3 + \phi_4) + O(h).$$

On the other hand, if one uses the cubic approximation, only $O(1)$ truncation error results, and still worse truncation errors are obtained by using the quadratic approximation. The quintic approximation yields an $O(h^2)$ truncation error, consistent with the truncation error obtained at interior nodes belonging to S_2 . However, this approximation requires a larger stencil, which yields in turn slightly irregular pentadiagonal matrices.

5. Calculation of the Stresses and Strains. In this section we discuss the explicit numerical computations of the stress components $\{\sigma_1, \sigma_2, \sigma_3\}$, and $\{\sigma_4, \sigma_5\}$ at each point in the computational grid from the potential functions ϕ and ψ , respectively. The stress component σ_3 is given, using (3.17), by $\sigma_3 = -\frac{1}{s_{33}}(\sigma_{31}\sigma_1 + \sigma_{32}\sigma_2 + \sigma_{34}\sigma_4 + \sigma_{35}\sigma_5 + \sigma_{36}\sigma_6)$. The strain vector ϵ is related linearly to the stresses vector and the temperature through Hooke's Law and is thus readily calculated once the stresses are known pointwise.

Recall that the stress components are defined on the domain Ω in terms of the potentials ϕ and ψ as follows:

$$\begin{aligned}\sigma_1 &= \frac{\partial^2 \phi}{\partial y^2} & \sigma_2 &= \frac{\partial^2 \phi}{\partial x^2} & \sigma_6 &= -\frac{\partial^2 \phi}{\partial x \partial y} \\ \sigma_5 &= \frac{\partial \psi}{\partial y} & \sigma_4 &= -\frac{\partial \psi}{\partial x}.\end{aligned}\quad (5.1)$$

By performing the transformation, $(x, y) \mapsto (\xi, \eta) \equiv ((x - y \cot \alpha)/a, y/b)$, which maps Ω onto the unit square Γ , it is easily verified that equations (5.1) become

$$\begin{aligned}\sigma_1 &= \frac{1}{b^2} \frac{\partial^2 \phi}{\partial \eta^2} - 2 \frac{\cot \alpha}{ab} \frac{\partial^2 \phi}{\partial \xi \partial \eta} + \frac{\cot^2 \alpha}{a^2} \frac{\partial^2 \phi}{\partial \xi^2}, \\ \sigma_6 &= -\frac{1}{ab} \frac{\partial^2 \phi}{\partial \xi \partial \eta} + \frac{\cot \alpha}{a^2} \frac{\partial^2 \phi}{\partial \xi^2}, \\ \sigma_2 &= \frac{1}{a^2} \frac{\partial^2 \phi}{\partial \xi^2}, \\ \sigma_4 &= -\frac{1}{a} \frac{\partial \psi}{\partial \xi}, \\ \sigma_5 &= -\frac{\cot \alpha}{a} \frac{\partial \psi}{\partial \xi} + \frac{1}{b} \frac{\partial \psi}{\partial \eta}.\end{aligned}\quad (5.2)$$

The stress vector components can then be determined once all of the second partials of ϕ and first partials of ψ have been calculated at each grid point on the unit square.

For any interior grid point, $P(i, j) \in S_2$ (See definition in Sec. 4), the following fourth-order-accurate * discretization formulae are used for evaluating $\frac{\partial^2 \phi}{\partial \xi^2}$, $\frac{\partial^2 \phi}{\partial \eta^2}$, and $\frac{\partial^2 \phi}{\partial \xi \partial \eta}$:

$$\begin{aligned}\frac{\partial^2 \phi}{\partial \xi^2}(i, j) &= \frac{1}{12h^2}(-\phi(i-2, j) + 16\phi(i-1, j) - 30\phi(i, j) + 16\phi(i+1, j) - \phi(i+2, j)) \\ &\quad - \frac{1}{90}h^4 \frac{\partial^4 \phi}{\partial \xi^4}(i, j) + O(h^6),\end{aligned}\quad (5.3)$$

$$\begin{aligned}\frac{\partial^2 \phi}{\partial \eta^2}(i, j) &= \frac{1}{12k^2}(-\phi(i, j-2) + 16\phi(i, j-1) - 30\phi(i, j) + 16\phi(i, j+1) - \phi(i, j+2)) \\ &\quad - \frac{1}{90}k^4 \frac{\partial^4 \phi}{\partial \eta^4}(i, j) + O(k^6),\end{aligned}\quad (5.4)$$

* Although the numerical solutions obtained for ϕ are, at most, second-order-accurate, the numerical accuracy of derived stresses can be enhanced in some cases by the use of fourth-order-accurate discretizations. See, for example, the second sample problem in Section 7., where the numerical solution of ϕ is essentially exact.

$$\frac{\partial^2 \phi}{\partial \xi \partial \eta}(i, j) = \frac{1}{24hk} \begin{bmatrix} . & 1 & . & -1 & . \\ 1 & -10 & . & 10 & -1 \\ . & . & . & . & . \\ -1 & 10 & . & -10 & 1 \\ . & -1 & . & 1 & . \end{bmatrix} \phi(i, j) - \frac{h^4}{30} \frac{\partial^6 \phi}{\partial \xi^6}(i, j) - \frac{k^4}{30} \frac{\partial^6 \phi}{\partial \eta^6}(i, j) - \frac{h^2 k^2}{36} \frac{\partial^6 \phi}{\partial \xi^3 \partial \eta^3}(i, j) + O(h^6 + k^6). \quad (5.5)$$

For those grid points belonging to the set S_1 , some of the points in the corresponding stencils lie outside the logical grid. At these exterior points ϕ can be defined by any of the extrapolation formulæ given in (4.4)-(4.13). Of course, the truncation error estimates should be adjusted according to the choice made.

The evaluation of $\frac{\partial^2 \phi}{\partial \xi^2}$, $\frac{\partial^2 \phi}{\partial \eta^2}$, and $\frac{\partial^2 \phi}{\partial \xi \partial \eta}$ at boundary grid points $P(i, j) \in S_0$ is considered next. Here one takes advantage of the fact that both ϕ and its normal derivative ϕ_n vanish on Γ . It follows that on horizontal boundaries $\frac{\partial^2 \phi}{\partial \xi \partial \eta}$ and $\frac{\partial^2 \phi}{\partial \eta^2}$ vanish identically - and hence only the term $\frac{\partial^2 \phi}{\partial \xi^2}$ requires computation there. Similarly, one needs to compute only $\frac{\partial^2 \phi}{\partial \eta^2}$ on vertical boundaries. One can continue using the approximations (5.3) and (5.4) for all points of S_0 except for corner points. At corner points, the normal is obviously not defined; nevertheless, we will attempt to approximate the stresses there by using the (formally) second-order-accurate scheme

$$\begin{aligned} \frac{\partial^2 \phi}{\partial \xi^2}(i, j) &= \frac{1}{h^2} (\phi(i-1, j) - 2\phi(i, j) + \phi(i+1, j)) + O(h^2), \\ \frac{\partial^2 \phi}{\partial \eta^2}(i, j) &= \frac{1}{k^2} (\phi(i, j-1) - 2\phi(i, j) + \phi(i, j+1)) + O(k^2). \end{aligned} \quad (5.6)$$

For the discretization of the partial derivative ψ_ξ , one can use the center difference scheme

$$\frac{\partial \psi}{\partial \xi}(i, j) = \frac{1}{2h} (\psi(i+1, j) - \psi(i-1, j)) - \frac{h^2}{6} \frac{\partial^3 \psi}{\partial \xi^3}(i, j) + O(h^4). \quad (5.7)$$

By using equation (4.1) in (5.7), the following fourth-order-accurate difference scheme can also be used

$$\frac{\partial \psi}{\partial \xi}(i, j) = \frac{1}{12h} (-\psi(i+2, j) + 8\psi(i+1, j) - 8\psi(i-1, j) + \psi(i-2, j)) + O(h^4). \quad (5.8)$$

Similar expressions are obtained for ψ_η . When computing σ_4 , and σ_5 at boundary nodes, one should, once again, take advantage of the fact that ψ vanishes there.

6. Explicit Calculation of Material Displacements. The expression for the displacement vector (u, v, w) is derived here in closed form, assuming that the strain components $\{\epsilon_1, \epsilon_2, \epsilon_6\}$ and $\{\epsilon_4, \epsilon_5\}$ are given everywhere in the closure of Ω . (Recall that $\epsilon_3 = 0$.) With this derived expression we will then illustrate how the numerical values of (u, v, w) are calculated at all grid points from the values of the strain components at those grid points.

The displacement vector (u, v, w) is obtained at all points (x, y) in Ω by solving the system (3.17) of first order PDE's:

$$\frac{\partial u}{\partial x} = \epsilon_1, \quad (6.1a)$$

$$\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = \epsilon_6, \quad (6.1b)$$

$$\frac{\partial v}{\partial y} = \epsilon_2, \quad (6.1c)$$

$$\frac{\partial w}{\partial y} = \epsilon_4, \quad (6.1d)$$

$$\frac{\partial w}{\partial x} = \epsilon_5. \quad (6.1e)$$

In order to simplify the integration of equations (6.1), the parallelogram Ω is mapped, as usual, onto the unit square Γ , and equations (6.1a)–(6.1e) become:

$$\frac{\partial u}{\partial \xi} = \epsilon'_1, \quad (6.2a)$$

$$\frac{a}{b} \frac{\partial u}{\partial \eta} + \frac{\partial v}{\partial \xi} = \epsilon'_6, \quad (6.2b)$$

$$\frac{\partial}{\partial \eta}(v + \cot \alpha u) = \epsilon'_2, \quad (6.2c)$$

$$\frac{\partial w}{\partial \eta} = \epsilon'_4, \quad (6.2d)$$

$$\frac{\partial w}{\partial \xi} = \epsilon'_5, \quad (6.2e)$$

where

$$\begin{aligned} \epsilon'_1 &= a\epsilon_1, \\ \epsilon'_6 &= a(\epsilon_6 + \cot \alpha \epsilon_1), \\ \epsilon'_2 &= b(\epsilon_2 + \cot \alpha \epsilon_6 + \cot^2 \alpha \epsilon_1), \\ \epsilon'_4 &= b(\epsilon_4 + \cot \alpha \epsilon_5), \\ \epsilon'_5 &= a\epsilon_5. \end{aligned} \quad (6.2f)$$

Another transformation on the dependent variables $(u, v) \mapsto (\tilde{u}, \tilde{v})$, where

$$\tilde{u} = \frac{a}{b}u \quad \text{and} \quad \tilde{v} = v + \cot \alpha u, \quad (6.3)$$

reduces equations (6.2a)–(6.2c) to the standard form of (6.1a)–(6.1c); namely,

$$\frac{\partial \tilde{u}}{\partial \xi} = \tilde{\epsilon}_1, \quad (6.4a)$$

$$\frac{\partial \tilde{u}}{\partial \eta} + \frac{\partial \tilde{v}}{\partial \xi} = \tilde{\epsilon}_0, \quad (6.4b)$$

$$\frac{\partial \tilde{v}}{\partial \eta} = \tilde{\epsilon}_2, \quad (6.4c)$$

where,

$$\begin{aligned} \tilde{\epsilon}_1 &= \frac{a}{b} \epsilon'_1, \\ \tilde{\epsilon}_0 &= \epsilon'_0 + \cot \alpha \epsilon'_1, \\ \tilde{\epsilon}_2 &= \epsilon'_2. \end{aligned} \quad (6.5)$$

Integration of (6.4a) with respect to ξ , and of (6.4c) with respect to η (taking any fixed point (ξ_0, η_0) inside the unit square to be the lower limit of integration), gives the expressions

$$\tilde{u}(\xi, \eta) = \int_{\xi_0}^{\xi} \tilde{\epsilon}_1(s, \eta) ds + \tilde{u}(\xi_0, \eta), \quad (6.6)$$

$$\tilde{v}(\xi, \eta) = \int_{\eta_0}^{\eta} \tilde{\epsilon}_2(\xi, t) dt + \tilde{v}(\xi, \eta_0). \quad (6.7)$$

From (6.6) and (6.7) it is clear that the displacements $\tilde{u}(\xi, \eta)$ and $\tilde{v}(\xi, \eta)$ are completely determined once $\tilde{u}(\xi_0, \eta)$ and $\tilde{v}(\xi, \eta_0)$ have been found. To this end (6.4b) is integrated with respect to η , and the resulting expression is evaluated at $\xi = \xi_0$. One obtains

$$\tilde{u}(\xi_0, \eta) = \tilde{u}(\xi_0, \eta_0) - \int_{\eta_0}^{\eta} \frac{\partial \tilde{v}}{\partial \xi}(\xi_0, t) dt + \int_{\eta_0}^{\eta} \tilde{\epsilon}_0(\xi_0, t) dt. \quad (6.8)$$

But it follows from (6.7) that

$$\frac{\partial \tilde{v}}{\partial \xi}(\xi_0, t) = \int_{\eta_0}^t \frac{\partial \tilde{\epsilon}_2}{\partial \xi}(\xi_0, t') dt' + \frac{\partial \tilde{v}}{\partial \xi}(\xi_0, \eta_0), \quad (6.9)$$

and upon substituting (6.9) into (6.8) the desired expression for $\tilde{u}(\xi_0, \eta)$ is obtained; namely

$$\tilde{u}(\xi_0, \eta) = \tilde{u}(\xi_0, \eta_0) - \int_{\eta_0}^{\eta} \int_{\eta_0}^t \frac{\partial \tilde{\epsilon}_2}{\partial \xi}(\xi_0, t') dt' dt + \int_{\eta_0}^{\eta} \tilde{\epsilon}_0(\xi_0, t) dt - \frac{\partial \tilde{v}}{\partial \xi}(\xi_0, \eta_0)(\eta - \eta_0). \quad (6.10)$$

The expression for $\tilde{v}(\xi, \eta_0)$ is derived similarly from equations (6.4b) and (6.6), or more directly from (6.10) by observing that the transformations $(\tilde{u}, \tilde{v}) \mapsto (\tilde{v}, \tilde{u})$, $(\xi, \eta) \mapsto (\eta, \xi)$, and $(\tilde{\epsilon}_1, \tilde{\epsilon}_2) \mapsto (\tilde{\epsilon}_2, \tilde{\epsilon}_1)$ leave equations (6.4a)–(6.4c) invariant. It follows that

$$\tilde{v}(\xi, \eta_0) = \tilde{v}(\xi_0, \eta_0) - \int_{\xi_0}^{\xi} \int_{\xi_0}^s \frac{\partial \tilde{\epsilon}_1}{\partial \eta}(s', \eta_0) ds' ds + \int_{\xi_0}^{\xi} \tilde{\epsilon}_0(s, \eta_0) ds - \frac{\partial \tilde{u}}{\partial \eta}(\xi_0, \eta_0)(\xi - \xi_0). \quad (6.11)$$

It is useful to introduce here the following notation:

$$\left. \begin{aligned} E_1(\xi, \eta) &= \int_{\xi_0}^{\xi} \tilde{\epsilon}_1(s, \eta) ds, \\ E_2(\xi, \eta) &= \int_{\eta_0}^{\eta} \tilde{\epsilon}_2(\xi, t) dt, \\ F_1(\xi) &= \int_{\xi_0}^{\xi} \tilde{\epsilon}_0(s, \eta_0) ds, \\ F_2(\eta) &= \int_{\eta_0}^{\eta} \tilde{\epsilon}_0(\xi_0, t) dt, \\ G_1(\xi) &= \int_{\xi_0}^{\xi} \int_{\xi_0}^s \frac{\partial \tilde{\epsilon}_1}{\partial \eta}(s', \eta_0) ds' ds \\ &= \int_{\xi_0}^{\xi} (\xi - s') \frac{\partial \tilde{\epsilon}_1}{\partial \eta}(s', \eta_0) ds', \\ G_2(\eta) &= \int_{\eta_0}^{\eta} \int_{\eta_0}^t \frac{\partial \tilde{\epsilon}_2}{\partial \xi}(\xi_0, t') dt' dt \\ &= \int_{\eta_0}^{\eta} (\eta - t') \frac{\partial \tilde{\epsilon}_2}{\partial \xi}(\xi_0, t') dt'. \end{aligned} \right\} \quad (6.12)$$

It then follows from (6.6), (6.7), (6.10), and (6.11) that

$$\tilde{u}(\xi, \eta) = E_1(\xi, \eta) + F_2(\eta) - G_2(\eta) - \frac{\partial \tilde{v}}{\partial \xi}(\xi_0, \eta_0)(\eta - \eta_0), \quad (6.13)$$

$$\tilde{v}(\xi, \eta) = E_2(\xi, \eta) + F_1(\xi) - G_1(\xi) - \frac{\partial \tilde{u}}{\partial \eta}(\xi_0, \eta_0)(\xi - \xi_0). \quad (6.14)$$

Similarly, by integrating (6.2d) and (6.2e) one obtains

$$w(\xi, \eta) = \int_{\xi_0}^{\xi} \epsilon'_5(s, \eta) ds + \int_{\eta_0}^{\eta} \epsilon'_4(\xi_0, t) dt + w(\xi_0, \eta_0). \quad (6.15)$$

Without loss of generality it can be assumed that zero rigid body translation occurs relative to the original domain Ω . We therefore choose $u(\xi_0, \eta_0) = v(\xi_0, \eta_0) = w(\xi_0, \eta_0) = 0$ and by (6.3) it follows that

$$\tilde{u}(\xi_0, \eta_0) = \tilde{v}(\xi_0, \eta_0) = 0. \quad (6.16)$$

The remaining two constants $\frac{\partial \tilde{u}}{\partial \eta}(\xi_0, \eta_0)$ and $\frac{\partial \tilde{v}}{\partial \xi}(\xi_0, \eta_0)$, are determined by assuming zero rigid body rotation occurs relative to Ω . One can then choose that $\frac{\partial u}{\partial x}(x_0, y_0) = 0$, where (x_0, y_0) is the inverse image of (ξ_0, η_0) . This implies that $\partial v / \partial \xi$ also vanishes at (ξ_0, η_0) , and hence by (6.3) and (6.4), it follows that

$$\frac{\partial \tilde{v}}{\partial \xi}(\xi_0, \eta_0) = \cot \alpha \frac{b}{a} \tilde{\epsilon}_1(\xi_0, \eta_0) = \cot \alpha \epsilon'_1(\xi_0, \eta_0). \quad (6.17)$$

It also follows from equations (6.4c) and (6.17) that

$$\frac{\partial \tilde{u}}{\partial \eta}(\xi_0, \eta_0) = \tilde{\epsilon}_0 - \cot \alpha \frac{b}{a} \tilde{\epsilon}_1(\xi_0, \eta_0) = \epsilon'_0(\xi_0, \eta_0). \quad (6.18)$$

Finally by combining equations (6.3) and (6.13)–(6.18) the displacements $u(\xi, \eta)$, $v(\xi, \eta)$, and $w(\xi, \eta)$ are given by:

$$u(\xi, \eta) = \frac{b}{a} (E_1(\xi, \eta) + F_2(\eta) - G_2(\eta)) - \cot \alpha \epsilon_1(\eta - \eta_0), \quad (6.19)$$

$$v(\xi, \eta) = E_2(\xi, \eta) + F_1(\xi) - G_1(\xi) - \epsilon'_6(\xi_0, \eta_0)(\xi - \xi_0) - \cot \alpha u(\xi, \eta), \quad (6.20)$$

$$w(\xi, \eta) = \int_{\xi_0}^{\xi} \epsilon'_5(s, \eta) ds + \int_{\eta_0}^{\eta} \epsilon'_4(\xi_0, t) dt. \quad (6.21)$$

The displacements at grid points can be computed numerically by simply evaluating the integrals in equations (6.12) using some suitable quadrature formulae. Two quadrature formulae are used in the present work. The first quadrature expression is the second-order-accurate (locally third-order-accurate) trapezoidal rule,

$$\int_0^h f(s) ds = \frac{h}{2} (f(0) + f(h)) + O(h^3), \quad (6.22)$$

with a leading truncation error term of $-\frac{h^3}{12} f''(0)$. The second quadrature expression is the fourth-order-accurate formula

$$\int_0^h f(s) ds = \frac{h}{2} (f(0) + f(h)) + \frac{h^2}{12} (f'(0) - f'(h)) + O(h^5), \quad (6.23)$$

with a leading truncation error term of $\frac{h^5}{720} f''''(0)$. On the lower boundary, $f'(0)$ is usually not defined; and one can use instead of (6.23) the third-order-accurate formula

$$\int_0^h f(s) ds = \frac{h}{3} (f(0) + 2f(h)) - \frac{h^2}{6} f'(h) + O(h^4). \quad (6.24)$$

Similarly, on the upper boundary one can use instead of (6.23) the formula

$$\int_0^h f(s) ds = \frac{h}{3} (2f(0) + f(h)) + \frac{h^2}{6} f'(0) + O(h^4). \quad (6.25)$$

Remarks:

1. In equations (6.23)–(6.25) the same orders of accuracy hold if the derivatives $f'(0)$ and $f'(h)$ are replaced by center differences.
2. If an integrand involves the derivative of some function (such as the case with the functions G_1 and G_2 on equations (6.12)), we use only the trapezoidal rule because center differencing of the integrand and use of the higher-order-accurate formula would yield only a second (not fourth)-order-accurate formula.
3. In actual calculations, the fixed point (ξ_0, η_0) is chosen to be the center of the unit square. In contrast to choosing (ξ_0, η_0) as a boundary node, our choice results in a smaller discretization error in the approximation of G_1 and G_2 . Of course, if a boundary node (ξ_1, η_1) (whose inverse image in

the x - y plane is (x_1, y_1) is required to have zero motion, then the corresponding displacements u', v' are obtained from u, v through the relations

$$u'(x, y) = u(x, y) - u(x_1, y_1) - \omega(y - y_1),$$

$$v'(x, y) = v(x, y) - v(x_1, y_1) + \omega(x - x_1),$$

where, for example, $\omega = \frac{\partial u}{\partial y}(x_1, y_1)$, or $\omega = \frac{\partial v}{\partial x}(x_1, y_1)$.

7. Test Problems.

The PDE solution methods described above have been tested extensively from both physical and mathematical points of view. We present in this section two of the sample problems which have been used in these verifications. (Additional examples can be found in Reference 10.) The first sample problem has been formulated in order to provide sufficient numerical tests of a problem with known analytical solutions. We show both the development of the analytic solutions for the posed PDE problems and the numerical solutions obtained by the DADI solution method. This first sample problem is purposefully intended to be more demanding mathematically and numerically than it is physically. The second sample problem considers more physically interesting thermoelastic effects in an anisotropic crystal for which analytic solutions are generally unavailable.

Sample Problem 1. Some Test Problems with Known Analytic Solutions

We develop first the rationale by which one can formulate a set of test problems which have known analytic solutions. After developing this analytic "machinery", numerical solutions are then compared with the analytic solutions of one of the more demanding (trigonometric) test problems in order to verify the stability, convergence efficiency, and local truncation error properties of the numerical PDE solution method.

For the sake of convenience we consider the single potential equation (3.35). We choose a potential ϕ which satisfies the boundary conditions (3.36) and a source s such that $s = \tilde{L}_4\phi$. One is usually able to choose a potential ϕ so that it is possible to derive explicitly some particular solution for the temperature which satisfies the equation $\tilde{M}_2T = s$. The following list of potentials clearly satisfies the boundary condition (3.36), and the corresponding sources are such that a particular solution for the temperature can be obtained in closed form:

$$\left. \begin{aligned} \phi_1 &= (x(1-x)y(1-y))^2, \\ \phi_2 &= (1 - \cos(2\pi x))(1 - \cos(2\pi y)), \\ \phi_3 &= (x(1-x))^2(1 - \cos(2\pi y)), \\ \phi_4 &= (1 - \cos(2\pi x))(y(1-y))^2, \\ \phi_5 &= \sum_i c_i \phi_i, \end{aligned} \right\} \quad (7.1)$$

where the coefficients $c_i, i = 1, \dots, 5$ are constants. The fifth potential, which is a linear combination of the previous four potentials, is especially interesting because it is a non-separable one.

It is a straight forward matter to compute source functions, s_1, s_2, s_3, s_4 , and s_5 , which are generated by the potentials $\phi_1, \phi_2, \phi_3, \phi_4$, and ϕ_5 , respectively. Since we will present numerical results for the second potential, the corresponding source s_2 is written out explicitly as:

$$\begin{aligned} s_2 &= -(2\pi)^4 (a_{40} \cos(2\pi x) + a_{04} \cos(2\pi y) - (a_{40} + a_{22} + a_{04}) \cos(2\pi x) \cos(2\pi y) \\ &\quad + (a_{31} + a_{13}) \sin(2\pi x) \sin(2\pi y)) \end{aligned} \quad (7.2)$$

The following two claims are useful in deriving temperature functions corresponding to sources generated by (7.1):

Claim 1. Let n be a positive integer and f be a given integrable function. Then, a particular solution to the PDE

$$a_{20} \frac{\partial^2 T}{\partial x^2} + a_{11} \frac{\partial^2 T}{\partial x \partial y} + a_{02} \frac{\partial^2 T}{\partial y^2} = y^n f(x), \quad (7.3)$$

is given by

$$T = \sum_{i=0}^n C_i y^{n-i} f_{i+2}(x), \quad (7.4)$$

where $f_i(x)$ is an antiderivative of $f_{i-1}(x)$, $f_0(x) = f(x)$. The coefficients C_i are determined by the recursive relationship,

$$\left. \begin{aligned} C_i &= -(n-i+1)/a_{20} (a_{11} C_{i-1} + (n-i+2)a_{02} C_{i-2}), \quad i = 2, \dots, n \\ C_0 &= 1/a_{20} \\ C_1 &= -na_{11}/a_{20}^2. \end{aligned} \right\} \quad (7.5)$$

Proof. Direct substitution of (7.4) into (7.3) gives

$$\begin{aligned} \sum_{i=0}^n a_{20} C_i y^{n-i} f_i(x) + \sum_{i=0}^{n-1} a_{11} C_i (n-i) y^{n-i-1} f_{i+1}(x) + \sum_{i=0}^{n-2} a_{02} C_i (n-i)(n-i-1) y^{n-i-2} f_{i+2}(x) \\ = y^n f(x) \end{aligned} \quad (7.6)$$

which can be rewritten as

$$\begin{aligned} \sum_{i=0}^n a_{20} C_i y^{n-i} f_i(x) + \sum_{i=1}^n a_{11} C_{i-1} (n-i+1) y^{n-i} f(x) + \sum_{i=2}^n a_{02} C_{i-2} (n-i+2)(n-i+1) y^{n-i} f_i(x) \\ = y^n f(x). \end{aligned} \quad (7.7)$$

Equating to zero the coefficient of $y^{n-i} f_i$, $i = 0, \dots, n$ in the identity (7.7), the recursive relation (7.5) follows.

Claim 2. A particular solution to the PDE

$$a_{20} \frac{\partial^2 T}{\partial x^2} + a_{11} \frac{\partial^2 T}{\partial x \partial y} + a_{02} \frac{\partial^2 T}{\partial y^2} = e^{i\tau y} f(x) \quad (7.8)$$

is given by

$$T = e^{i\tau y} (T_1(x) + T_2(x)), \quad (7.9)$$

where

$$T_1 = C_1 e^{-\tau^2 x} \int e^{\tau^2 z} f(z) dz \quad (7.10)$$

$$T_2 = C_2 e^{-\tau^2 x} \int e^{\tau^2 z} f(z) dz \quad (7.11)$$

$$\left. \begin{aligned} r_1 &= ia + b, \\ r_2 &= ia - b, \\ a &= qa_{11}/2a_{20}, \\ b &= \frac{q}{a_{20}} \sqrt{a_{20}a_{02} - \left(\frac{a_{11}}{2}\right)^2}, \\ C_1 &= -1/(4a_{20}b), \\ C_2 &= -C_1 \end{aligned} \right\} \quad (7.12)$$

Proof. Direct differentiation of (7.10) yields

$$\begin{aligned} \frac{\partial T_1}{\partial x} &= -r_1 T_1 + C_1 f(x), \\ \frac{\partial^2 T_1}{\partial x^2} &= r_1^2 T_1 - 2r_1 C_1 f(x) + C_1 f'(x). \end{aligned}$$

Similar expressions are obtained by differentiating (7.11). By substitution in (7.8), it follows that

$$\begin{aligned} a_{20}T_{xx} + a_{11}T_{xy} + a_{02}T_{yy} &= e^{iqy} \left(a_{20}(r_1^2 T_1 + r_2^2 T_2 - 2(r_1 C_1 + r_2 C_2)f + (C_1 + C_2)f') \right. \\ &\quad \left. + iq a_{11}(-r_1 T_1 - r_2 T_2 + (C_1 + C_2)f) - a_{02}q^2(T_1 + T_2) \right) = e^{iqy} f \end{aligned}$$

The above identity will be satisfied for all x and y if the following conditions are met:

(1) r_1 and r_2 are the zeroes of the characteristic equation

$$a_{20}r^2 - iq a_{11}r - a_{02}q^2 = 0,$$

(2) $-2a_{20}(r_1 C_1 + r_2 C_2) + iq a_{11}(C_1 + C_2) = 1$,

(3) $C_1 + C_2 = 0$.

Clearly, (1), (2), and (3) are equivalent to (7.12).

Corollary 1. Assuming that $(a_{20} + a_{02})^2 - a_{11}^2 \neq 0$, then

(i) for $f(x) = \cos(qx)$ in (7.8), the following particular solution is obtained:

$$T = -\frac{e^{iqy}}{q^2((a_{20} + a_{02})^2 - a_{11}^2)} ((a_{20} + a_{02}) \cos(qx) - ia_{11} \sin(qx)).$$

Consequently, the real part of T ,

$$\Re T = \frac{-1}{q^2((a_{20} + a_{02})^2 - a_{11}^2)} ((a_{20} + a_{02}) \cos(qx) \cos(qy) + a_{11} \sin(qx) \sin(qy)),$$

is a solution of (7.8) with right hand side equal to $\cos(qx) \cos(qy)$. Similarly, the imaginary part of T ,

$$\Im T = \frac{-1}{q^2((a_{20} + a_{02})^2 - a_{11}^2)} ((a_{20} + a_{02}) \cos(qx) \sin(qx) - a_{11} \sin(qx) \cos(qy)).$$

is a solution of (7.8) with right hand side equal to $\cos(qx)\sin(qy)$.

(ii) The case $f(x) = \sin(qx)$ is obtained from (i) by replacing x with $x - \pi/2q$. As a result, the expressions

$$\Re T = \frac{-1}{q^2((a_{20} + a_{02})^2 - a_{11}^2)} ((a_{20} + a_{02})\sin(qx)\cos(qy) - a_{11}\cos(qx)\sin(qy)),$$

and

$$\Im T = \frac{-1}{q^2((a_{20} + a_{02})^2 - a_{11}^2)} ((a_{20} + a_{02})\sin(qx)\sin(qy) + a_{11}\cos(qx)\cos(qy)),$$

are solutions to (7.8) with right hand sides equal to $\sin(qx)\cos(qy)$ and $\sin(qx)\sin(qy)$ respectively.

(iii) Provided that $a_{02} \neq 0$, the trivial case $f(x) = 1$ yields

$$T = \frac{-e^{iqy}}{a_{02}q^2}.$$

Proof. Using the results of claim 2, with $f(x) = \cos(qx)$, it follows that:

$$T_1 = C_1(r_1 \cos(qx) + q \sin(qx)) / (r_1^2 + q^2)$$

$$T_2 = -C_1(r_2 \cos(qx) + q \sin(qx)) / (r_2^2 + q^2).$$

Also, by using the identities

$$r_1 r_2 = -a_{02}q^2/a_{20},$$

$$r_1 + r_2 = iq a_{11}/a_{20},$$

$$r_1 - r_2 = 2b,$$

the above corollary can be established.

Remarks:

1. The restrictions on the coefficients a_{20} , a_{11} , and a_{02} are obviously met if (7.6) is elliptic.
2. The results in corollary 1 can be obtained directly by using the method of undetermined coefficients.

Corollary 2. For an isotropic medium, assuming a potential solution is given by $\phi = \phi_2 = (1 - \cos 2\pi x)(1 - \cos 2\pi y)$, then a possible temperature distribution associated with this potential is given by

$$T = \frac{-(2\pi)^2}{\alpha E} (1 - \nu) (\cos 2\pi x + \cos 2\pi y - 2 \cos 2\pi x \cos 2\pi y). \quad (7.13)$$

Proof. From (3.42) it follows that T satisfies the Poisson equation

$$\nabla^2 T = \frac{(2\pi)^4}{\alpha E} (1 - \nu) (\cos 2\pi x + \cos 2\pi y - 4 \cos 2\pi x \cos 2\pi y). \quad (7.14)$$

Using the results of corollary 1 or by inspection, it follows that (7.13) is indeed a particular solution.

It is also easy to compute the displacements in closed form. Indeed, using (3.20), the stresses σ_1 , σ_2 , and σ_3 are given by

$$\begin{aligned}\sigma_1 &= (2\pi)^2 \cos 2\pi y (1 - \cos 2\pi x), \\ \sigma_2 &= (2\pi)^2 \cos 2\pi x (1 - \cos 2\pi y), \\ \sigma_3 &= - (2\pi)^2 \sin 2\pi x \sin 2\pi y.\end{aligned}\quad (7.15)$$

Substituting into (3.40), we obtain the following expressions for the strains:

$$\begin{aligned}\epsilon_1 &= -\frac{(2\pi)^2}{E} (1 + \nu) \cos 2\pi x (1 - \cos 2\pi y), \\ \epsilon_2 &= -\frac{(2\pi)^2}{E} (1 + \nu) \cos 2\pi y (1 - \cos 2\pi x), \\ \epsilon_3 &= -2\frac{(2\pi)^2}{E} (1 + \nu) \sin 2\pi x \sin 2\pi y.\end{aligned}\quad (7.16)$$

Notice that the displacements can then be obtained in closed form from (6.19) and (6.20):

$$\begin{aligned}u &= -\frac{2\pi}{E} (1 + \nu) \sin 2\pi x (1 - \cos 2\pi y), \\ v &= -\frac{2\pi}{E} (1 + \nu) \sin 2\pi y (1 - \cos 2\pi x).\end{aligned}\quad (7.17)$$

Numerical Results. Figure 7.1 shows the scaled temperature distribution on the unit square domain as given by equation (7.13) for an idealized isotropic material in which $E = 1$, $\nu = \frac{1}{4}$, $\alpha = 1$. Figure 7.2 presents the numerical solution for the stress potential ϕ which satisfies (3.42) with $\nabla^2 T$, appearing on the right-hand-side, being given by (7.14). Figures 7.3-7.5 present the derived solutions for the stress components σ_1 and σ_3 , and the displacement component u respectively. (The stress component σ_2 and the displacement component v are obtained from σ_1 and u , respectively, by simple rotation and thus are not shown graphically.) Figure 7.6 shows the displaced grid in some appropriately chosen units. It is interesting to note that, in this example, the displacements at the boundary are zero to within arbitrary rigid body motion, even though free-surface boundary conditions were applied. This result is somewhat paradoxical because the solutions of the free-surface boundary value problem also happened to be the solution of the clamped boundary value problem. Comparison of the numerically computed stress potential to the exact solution, as given by the function ϕ_2 in equation (7.1), indicate that a relative error in the max norm (i.e., $\max|\phi_2 - \phi|/\max|\phi_2|$) of approximately .16% is incurred at the center of the square for a 65×65 grid. (See Table 1.) A sequence of calculations on a set of refined grids of sizes 9×9 , 17×17 , 33×33 , and 65×65 confirms that the error diminishes almost exactly as $O(h^2)$, in agreement with the truncation error estimate. The error properties of the numerically computed stresses, strains, and displacements are similar to those mentioned for the stress potential.

Percentage of Relative Error Norm in Grid Size	ϕ	σ_1	σ_6	ϵ_1	u	Number of DADI Steps
9 x 9	10.19	10.19	7.31	6.17	11.12	16
17 x 17	2.58	2.57	2.38	1.83	2.97	22
33 x 33	0.64	0.64	0.63	0.48	0.75	25
65 x 65	0.16	0.16	0.16	0.12	0.19	25

Table 1. Normalized maximum error norm in solutions computed in Sample Problem 1 for the variables indicated. The number of DADI steps required for achieving error norm less than 10^{-9} is displayed in the last column.

Figure 7.1 Scaled Temperature distribution on the unit square domain as given by equation (7.13).

Figure 7.2 Isocontours of the computed solution for the stress potential in sample problem 1.

Figure 7.3 Isocontours of the computed solution for the stress component σ_1 .

Figure 7.4 Isocontours of the computed solution for the stress component σ_0 .

Figure 7.5 Isocontours of the computed displacement component u .

Figure 7.6 Displaced grid. The new coordinates (U, V) of this displaced grid are given by $U(x, y) = x + \lambda u(x, y)$, $V(x, y) = y + \lambda v(x, y)$, x and y being the original coordinates of the undeformed grid, and λ is a scaling factor.

Sample Problem 2. Thermal Stress Effects in Trigonal Al_2O_3 Crystals with a Designated Polynomial Temperature Distribution.

Rectangular slabs of Al_2O_3 with a designated polynomial temperature distribution are considered in this example. By assuming the crystal slab surfaces to be cut in various orientations relative to the natural crystal axes, this sample problem will exhibit both purely planar (2-D) and generalized 3-D deformations of the trigonal Al_2O_3 crystal. In order to illustrate the sensitivity of anisotropic stresses, strains, and deformations to crystal shapes and orientations for a given crystal class with a given temperature distribution, three cases are examined for Al_2O_3 crystals.

The first case assumes that the rectangular crystal slab edges correspond completely to the conventional coordinate axes (x_1, x_2, x_3) as indicated in Figure 7.7. The (x, y, z) axes represent the laboratory frame which is used for physics computations.

Figure 7.7 Schematic representation of a rectangular parallelepiped slab of Al_2O_3 . The slab surface orientations are in complete correspondence to the conventional coordinate axes (x_1, x_2, x_3) in this case.

In order to model 3-D deformations reliably with computations which use only two spatial variables (x, y) it is assumed that: (i) the slab is unconstrained; (ii) the slab dimension in the z -direction is large compared to the x - and y - dimensions; and (iii) thermal loading in the slab is independent of z . We have arbitrarily elected to align the cross-sectional "width" of the slab with the x -axis and the cross sectional "height" with the y -axis. In this laboratory frame orientation, the non-zero elastic

compliance matrix elements for Al_2O_3 in the generalized Hooke's Law (3.11) are:

$$\begin{aligned}
 s_{11} &= s_{22} = 2.35 \times 10^{-13} \text{ cm}^2/\text{dyne} \\
 s_{33} &= 2.17 \times 10^{-13} \\
 s_{12} &= -0.72 \times 10^{-13} \\
 s_{13} &= s_{23} = -0.36 \times 10^{-13} \\
 s_{14} &= -s_{24} = 0.49 \times 10^{-13} \\
 s_{44} &= s_{55} = 6.94 \times 10^{-13} \\
 s_{56} &= 0.98 \times 10^{-13} \\
 s_{66} &= 6.14 \times 10^{-13}
 \end{aligned} \tag{7.18}$$

and the non-zero thermal expansion coefficients are

$$\begin{aligned}
 \alpha_1 &= \alpha_2 = 5.85 \times 10^{-6} (^\circ\text{K})^{-1} \\
 \alpha_3 &= 6.23 \times 10^{-6}
 \end{aligned} \tag{7.19}$$

The temperature distribution function is $T = 4y(1 - y)$; and, using $T_{\text{reference}} = T_{\text{average}}$, the temperature deviation function in the slab is $\delta T = 4y(1 - y) - \frac{2}{3}$ in all of the cases considered in this sample problem.

The stress potential equations (3.21)–(3.25) in the laboratory frame can now be solved for generalized plane deformation in this test case using the boundary conditions (3.29). The actual numerical PDE solution process is carried out on the unit square as defined by (3.30)–(3.34). From the computed stress potentials, material stresses are evaluated according to (5.1)–(5.8); the material strains are evaluated according to Hooke's Law; and material displacements are evaluated according to equations (6.3) and (6.19)–(6.21). Figure 7.8 presents a 3-D plot of the material displacements u , v , and w relative to the undeformed state in some scaled units on a 65×65 grid. These displacements, although functions of only the independent variables x and y , are clearly three-dimensional. The displacement w in the z -direction, is clearly a non-trivial function of x and y . This problem was run with both large and small grid meshes. The convergence properties were consistent with the local truncation error properties discussed previously. These solutions converged in fewer than 30 iterations. The CPU time on the LLNL Cray 1S computer was a fraction of a second for the largest mesh considered (81×81).

Figure 7.8 Two different viewing angles of the magnified material displacement surface for the first case of sample problem 2. This surface is drawn in the U, V, W space and is parameterized by the original coordinates (x, y) , where $U(x, y) = x + \lambda u(x, y)$, $V(x, y) = y + \lambda v(x, y)$, $W(x, y) = \mu w(x, y)$. The magnification factors λ and μ are given the values $\lambda = 10^5$ and $\mu = 50\lambda$.

The second case considers a rectangular crystal slab to be cut in an orientation in which the crystal has first been rotated by 90° about x_3 relative to the conventional orientation considered immediately above. Figure 7.9 represents the laboratory and crystal orientations for this case.

Figure 7.9 Schematic representation of a rectangular slab of Al_2O_3 in which the crystal's natural axes are rotated by 90° about x_3 , relative to case 1.

The temperature deviation function is again given by $\delta T = 4y(1-y) - \frac{2}{3}$, and the material stresses, strains, and deformations are computed in the same manner as in case 1. The material properties in the laboratory frame for this second case are obtained by transforming the elastic compliances and thermal expansion tensor according to the rules discussed in Appendix B. The transformed values are

$$\begin{aligned}
 s_{11} &= s_{22} = 2.35 \times 10^{-13} \text{ cm}^2/\text{dyne} \\
 s_{33} &= 2.17 \times 10^{-13} \\
 s_{12} &= -0.72 \times 10^{-13} \\
 s_{13} &= s_{23} = -0.36 \times 10^{-13} \\
 s_{15} &= -s_{25} = -0.49 \times 10^{-13} \\
 s_{44} &= s_{55} = 6.94 \times 10^{-13} \\
 s_{46} &= 0.98 \times 10^{-13} \\
 s_{66} &= 6.14 \times 10^{-13},
 \end{aligned} \tag{7.20}$$

and the thermal expansion coefficients are unchanged from the values given by (7.19) for the first case. The computed material displacements are shown in Figure 7.10. These displacements differ both qualitatively and quantitatively from the results computed in first case. The displacement in the z -direction is again a non-constant function of x and y .

Figure 7.10 Two different viewing angles of the magnified material displacement surface relative to the undeformed state for the second case of sample problem 2.

The third case considers the Al_2O_3 crystal to be rotated by 90° from its orientation in the second case above prior to cutting it into a rectangular slab. The orientation of laboratory and conventional coordinate axes in this case appears in Figure 7.11.

Figure 7.11. Schematic representation of a rectangular slab of Al_2O_3 in which the crystal's natural axes are rotated by 90° about x_1 , relative to case 2.

Application of the appropriate tensor transformations yields the following non-zero material properties in the laboratory frame for this third case.

$$\begin{aligned}
 s_{11} = s_{33} &= 2.35 \times 10^{-13} \text{ cm}^2/\text{dyne} \\
 s_{22} &= 2.17 \times 10^{-13} \\
 s_{12} = s_{23} &= -0.36 \times 10^{-13} \\
 s_{13} &= -0.72 \times 10^{-13} \\
 s_{16} = -s_{36} &= -0.49 \times 10^{-13} \\
 s_{44} = s_{66} &= 6.94 \times 10^{-13} \\
 s_{45} &= 0.98 \times 10^{-13} \\
 s_{55} &= 6.14 \times 10^{-13}
 \end{aligned} \tag{7.21}$$

and

$$\begin{aligned}
 \alpha_1 = \alpha_3 &= 5.85 \times 10^{-6} (^\circ\text{K})^{-1} \\
 \alpha_2 &= 6.23 \times 10^{-6}
 \end{aligned} \tag{7.22}$$

Figure 7.12 plots the computed material displacements. In this case the displacement w in the z -direction is a constant for all x, y . This purely planar displacement can be rationalized logically by first observing that in this case the compliance elements s_{m4} and s_{m5} and the thermal expansion

coefficients α_k are zero for $m = 1, 2, 3, 8$, and for $k = 4, 5$, and 6. From equations (3.21)–(3.24) and the boundary conditions (3.34) it follows that the potential ψ is identically zero; and hence by the defining relations (3.17) and (3.20) and Hooke's Law it follows that the displacement w is constant.

Figure 7.12 Magnified material displacement planar surface relative to the undeformed state for the third case of sample problem 2.

Conclusions

The DADI method has been developed and applied to the numerical solution of both the heat equation and an elliptic system of fourth-order PDE's which describe thermoelasticity in arbitrary crystal symmetry classes and thermal environments. Local truncation error properties of the different discretization schemes which were used have been theoretically derived and experimentally confirmed for temperatures, for stress potentials, and for the derived material stresses, strains, and displacements. Although this work has been limited at the present time to the study of the two-dimensional problem, the stress potential formulations and the DADI method presented in this work can be applied to treat also the case of a finite slab in 3-D.

Appendix A.

We consider here the effect of general coordinate rotation on the stress, strain, and compliance tensors. Equivalent expressions are also given in the compact matrix notation. In order to distinguish between the tensor and vector notation of the stresses and strains we use the original notation of section 3.A. Namely, we denote by σ^i and ϵ^i the stress and strain vectors, respectively, and by σ and ϵ the stress and strain tensors, respectively.

Definition and notation

Let $R = (r_{ij})$ denote that rotation matrix which relates the two orthogonal coordinate systems x_1, x_2, x_3 "old" and $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3$ "new". That is, if P is a point with vector position $x^i = (x_1, x_2, x_3)$ and $\tilde{x}^i = (\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)$ in the old and new coordinate systems, respectively, (the upper index i denotes the transpose of the quantity under consideration) then

$$\tilde{x} = R x. \quad (A.1)$$

The matrix R has the property that its transpose is equal to its inverse.

Hooke's Law, in the absence of temperature variation, is commonly written in tensor form by means of a fourth-rank compliance tensor s_{ijkl} , $1 \leq i, j, k, l \leq 3$, as

$$\epsilon_{pq} = s_{pqrs} \sigma_{rs}. \quad (A.2)$$

The tensor s_{ijkl} has the symmetry properties

$$\begin{aligned} s_{ijkl} &= s_{jikl}, \\ s_{ijkl} &= s_{ijlk}, \\ s_{ijkl} &= s_{klij}. \end{aligned} \quad (A.3)$$

The symmetry of the first two and last two indices permits one to write the tensor s_{ijkl} in the more compact six-by-six matrix notation $S = (s_{mn})$ of section 3. This is accomplished through the following convention:

$$\begin{array}{ll} \text{tensor (or long) notation} & ij \text{ or } kl = 11 \ 22 \ 33 \ 23 \ 31 \ 12 \\ \text{matrix (or short) notation} & m \text{ or } n = 1 \ 2 \ 3 \ 4 \ 5 \ 6 \end{array} \quad (A.4)$$

Because of the particular choice of the strain vector ϵ^i in (3.6), the following relations exist between the short and long notation, which in turn imply that S is symmetric:

$$s_{mn} = \begin{cases} s_{ijkl} & 1 \leq m, n \leq 3 \\ 2s_{ijkl} & 4 \leq \text{either } m \text{ or } n \leq 6 \\ 4s_{ijkl} & 4 \leq \text{both } m \text{ and } n \leq 6. \end{cases} \quad (A.5)$$

Henceforth, the symbol *tilde* attached to a quantity will indicate that this quantity is evaluated relative to the new coordinate system.

It is well-known that the relation between the stress tensors σ and $\bar{\sigma}$ is given by (see for example [8])

$$\bar{\sigma}_{ij} = r_{is} r_{jt} \sigma_{st}, \quad (\text{A.6})$$

or in matrix notation

$$\bar{\sigma} = R \sigma R^t. \quad (\text{A.7})$$

Similarly, the strain tensor ϵ_{ij} transforms as

$$\bar{\epsilon}_{ij} = r_{kp} r_{lq} \epsilon_{pq}, \quad (\text{A.8})$$

or in matrix form as

$$\bar{\epsilon} = R \epsilon R^t. \quad (\text{A.9})$$

It follows from (A.2) that

$$\bar{\epsilon}_{kl} = r_{kp} r_{lq} r_{is} r_{jt} s_{pqst} \bar{\sigma}_{ij}, \quad (\text{A.10})$$

which implies that the old compliance tensor s_{pqst} transforms to the new compliance tensor $\bar{s}_{klis}$ according to the relation

$$\bar{s}_{klis} = r_{kp} r_{lq} r_{is} r_{jt} s_{pqst}. \quad (\text{A.11})$$

The new tensor $\bar{s}_{klis}$ obviously satisfies the same symmetry properties (A.3) as the old tensor s_{pqst} .

Our next aim is to write out what is equivalent to the relationship (A.11) when the corresponding matrix representation is used, in such a way that symmetry is preserved.

Claim 1. The tensor relation (A.6) (or the equivalent matrix representation (A.7)) can be written in the following compact vector form:

$$\bar{\sigma}' = Q \sigma', \quad (\text{A.12})$$

where Q is the 6×6 matrix

$$Q = \begin{pmatrix} r_{11}^2 & r_{12}^2 & r_{13}^2 & 2r_{12}r_{13} & 2r_{13}r_{11} & 2r_{11}r_{12} \\ r_{21}^2 & r_{22}^2 & r_{23}^2 & 2r_{22}r_{23} & 2r_{23}r_{21} & 2r_{21}r_{22} \\ r_{31}^2 & r_{32}^2 & r_{33}^2 & 2r_{32}r_{33} & 2r_{33}r_{31} & 2r_{31}r_{32} \\ r_{21}r_{31} & r_{22}r_{32} & r_{23}r_{33} & r_{22}r_{33} + r_{23}r_{32} & r_{23}r_{31} + r_{21}r_{33} & r_{21}r_{32} + r_{22}r_{31} \\ r_{31}r_{11} & r_{32}r_{12} & r_{33}r_{13} & r_{32}r_{13} + r_{33}r_{12} & r_{33}r_{11} + r_{31}r_{13} & r_{31}r_{12} + r_{32}r_{11} \\ r_{11}r_{21} & r_{12}r_{22} & r_{13}r_{23} & r_{12}r_{23} + r_{13}r_{22} & r_{13}r_{21} + r_{11}r_{23} & r_{11}r_{22} + r_{12}r_{21} \end{pmatrix}. \quad (\text{A.13})$$

Furthermore, the inverse of Q is obtained from Q by replacing the factors r_{ij} by r_{ji} , $1 \leq i, j \leq 3$.

Proof. Equation (A.12) can readily be verified by inspection. The second part of the claim is established by noticing that σ in equation (A.7) can be expressed in terms of $\bar{\sigma}$ as

$$\sigma = R^t \bar{\sigma} R. \quad (\text{A.14})$$

Claim 2. The strain vector ϵ' transforms to $\bar{\epsilon}'$ according to the relation

$$\bar{\epsilon}' = (Q^{-1})^t \epsilon'. \quad (\text{A.15})$$

Proof: Let us write

$$\epsilon'' = (\epsilon_{11}, \epsilon_{22}, \epsilon_{33}, \epsilon_{23}, \epsilon_{31}, \epsilon_{12})^t,$$

and recall that

$$\begin{aligned}\epsilon' &= (\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5, \epsilon_6)^t, \\ &= (\epsilon_{11}, \epsilon_{22}, \epsilon_{33}, 2\epsilon_{23}, 2\epsilon_{31}, 2\epsilon_{12})^t,\end{aligned}$$

one can then write

$$\epsilon' = D\epsilon'',$$

where D is the diagonal matrix

$$D = \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 2 & & \\ & & & & 2 & \\ & & & & & 2 \end{pmatrix}.$$

Since ϵ'' transforms in exactly the same manner as σ' , i.e.,

$$\tilde{\epsilon}'' = Q\epsilon'',$$

it follows that

$$\tilde{\epsilon}' = DQD^{-1}\epsilon', \quad (\text{A.16})$$

which can be shown to be equivalent to (A.15).

Notice that (A.15) shows that $\tilde{\epsilon}'$ is not obtained from ϵ' by simply premultiplying ϵ' by Q as was found in the case of the stress vector transformation.

Corollary. The compliance matrices S and $\tilde{S}$ are related by

$$\tilde{S} = (Q^{-1})^t S Q^{-1}, \quad (\text{A.17})$$

and hence $\tilde{S}$ is also symmetric.

Proof: Recall that $\epsilon' = S\sigma'$, $\tilde{\epsilon}' = \tilde{S}\tilde{\sigma}'$, and using the relations (A.12) and (A.15), equation (A.17) follows.

Appendix B.

We wish to show here that the operators L_4 and L_2 of section 3 are elliptic operators. The proof is established solely on the basis that the compliance matrix $S = (s_{ij})$ is positive definite as follows.

Claim 1. *The polynomial*

$$\bar{L}_4(x, y) = s_{12}x^4 - 2s_{26}x^3y + (2s_{12} + s_{66})x^2y^2 - 2s_{16}xy^3 + s_{11}y^4 \quad (B.1)$$

is positive for all real x and y except $x = y = 0$.

Proof. Let z be the real vector

$$z = (z_1, z_2, 0, 0, 0, z_6)^t$$

then

$$(z, Sz) = s_{22}z_2^2 + 2s_{26}z_2z_6 + 2s_{12}z_1z_2 + s_{66}z_6^2 + 2s_{16}z_1z_6 + s_{11}z_1^2 \quad (B.2)$$

By comparing (B.1) and (B.2) it follows that, upon choosing

$$z_2 = x^2, \quad z_6 = -xy, \quad z_1 = y^2,$$

(B.2) reduces to (B.1) and hence the claimed result is obtained.

Claim 2. *The polynomial*

$$\bar{L}_2(x, y) = s_{44}x^2 - 2s_{45}xy + s_{55}y^2 \quad (B.3)$$

is positive for all real x and y except $x = y = 0$.

Proof. This result is established once z is chosen as

$$z = (0, 0, 0, x, -y, 0)^t.$$

The following claim extends the results of the previous claims to the case when the coefficients s_{ij} are replaced by s'_{ij} , where

$$s'_{ij} = s_{ij} - \frac{s_{i3}s_{3j}}{s_{33}} \quad (B.4)$$

Claim 3. *The reduced 5-by-5 symmetric matrix*

$$S' = \begin{pmatrix} s'_{11} & s'_{12} & s'_{14} & s'_{15} & s'_{16} \\ & s'_{22} & s'_{24} & s'_{25} & s'_{26} \\ & & s'_{44} & s'_{45} & s'_{46} \\ & & & s'_{55} & s'_{56} \\ & & & & s'_{66} \end{pmatrix} \quad (B.5)$$

is positive definite.

Proof. By choosing the vector $z = (z_1, z_2, z_3, z_4, z_5, z_6)^t$ such that

$$z_3 = -\frac{1}{s_{33}} \sum_{\substack{1 \leq i \leq 6 \\ i \neq 3}} s_{3i}z_i,$$

it is readily shown that

$$(z, Sz) = (z', S' z')$$

where z' is the reduced vector

$$z' = (z_1, z_2, z_4, z_5, z_6)$$

and hence the claimed result is obtained. The following corollary is an immediate result of claim 3.

Corollary. The operators L_2 and L_4 are *elliptic*.

Claim 4. The transformed operator L'_2 of equation (3.32) remains elliptic.

Proof. The characteristic polynomial associated with L'_2 is $A_{20}\xi^2 + A_{11}\xi\eta + A_{02}\eta^2$; and using equation (3.33) it follows that

$$\begin{aligned} & A_{20}\xi^2 + A_{11}\xi\eta + A_{02}\eta^2 \\ &= a_{20} \left(\frac{\xi}{a} \right)^2 + a_{11} \frac{\xi}{a} \left(\frac{\eta}{b} - \frac{\cot \alpha}{a} \xi \right) + a_{02} \left(\frac{\eta}{b} - \frac{\cot \alpha}{a} \xi \right)^2 \\ &\equiv a_{20} z_1^2 + a_{11} z_1 z_2 + a_{02} z_2^2. \end{aligned}$$

The last polynomial is the characteristic polynomial of the original elliptic operator L_2 , and hence L'_2 is elliptic.

Similarly, one can show that L'_4 is elliptic. It is also straight forward to show that these results hold true for any non-singular coordinate transformation.

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Appendix 2

3-D ELASTIC COMPLIANCE MATRIX STRUCTURES

Key to Notation

- zero component
 - non-zero component
 - equal components
 - components numerically equal, but opposite in sign
- For s ⊙ twice the numerical equal of the heavy dot component to which it is joined
- For c ⊙ the numerical equal of the heavy dot component to which it is joined
- For s x $2(s_{11} - s_{12})$
- For c x $\frac{1}{2}(c_{11} - c_{12})$

All the matrices are symmetrical about the leading diagonal.

Triclinic

Both Classes

(21 independent matrix elements)

Monoclinic

All Classes

(13 independent matrix elements)

Orthorhombic

All Classes

(9 independent matrix elements)

Cubic

All Classes

(3 independent matrix elements)

1

A 5x5 grid of dots. The dots are arranged in 5 rows and 5 columns. The following pairs of dots are connected by lines: (row, column) pairs (1,1)-(1,2), (1,3)-(1,4), (2,3)-(2,4), (3,4)-(3,5), (4,2)-(4,3), and (5,4)-(5,5). The entire grid is enclosed in large parentheses.

All Classe

A 5x5 grid of dots. A path of 5 black dots starts at (1,1), goes to (1,2), then (2,2), then (2,3), and ends at (3,3). A path of 3 white dots starts at (4,4), goes to (4,5), and ends at (5,5). The paths do not intersect.

Appendix 3

MATERIAL DATA FOR CODE VALIDATIONS

The selection of representative crystalline materials for thermal stress code validations is somewhat limited because of the scarcity of simultaneous data for thermal conductivities, expansion coefficients and elastic compliance matrix elements. Those materials for which reasonably comprehensive data presently exists for code benchmarking includes the following crystal systems and materials:

Cubic:	$Y_3Al_5O_{12}$	(YAG)
Trigonal:	Al_2O_3	(Alumina, Corundum)
Tetragonal:	KH_2PO_4	(KDP)
Hexagonal:	SiO_2	(β - quartz)
Orthorhombic:	$CaCO_3$	(Aragonite)

Available data for thermal conductivities, thermal expansion ratios, and elastic compliance and stiffness constants are tabulated in Table 3.1.

TABULATION OF SELECTED THERMOELASTIC MATERIAL PROPERTIES

Crystal Material	Thermal Conductivity erg/(cm ² K)	Thermal Expansion Ratio (°K) ⁻¹	Elastic Compliances (cm ² /dyne)	Elastic Stiffnesses (dyne/cm ²)	Elasto-Optic Coefficients (Dimensionless)
Y ₃ Al ₅ O ₁₂ (Cubic) See Reference 14 for all material properties	1.1x10 ⁶ with Nd ³⁺ 1 atomic percent	6.96x10 ⁻⁶	$s_{11}=s_{22}=s_{33}=3.59 \times 10^{-13}$ $s_{12}=s_{13}=s_{23}=-.90 \times 10^{-13}$ $s_{66}=s_{44}=8.69 \times 10^{-13}$	$c_{11}=c_{22}=c_{33}=3.33 \times 10^{12}$ $c_{12}=c_{13}=c_{23}=1.1 \times 10^{12}$ $c_{66}=c_{44}=1.15 \times 10^{12}$	$p_{11}=p_{22}=p_{33}=-.29$ $p_{12}=.0091$ $p_{66}=p_{44}=-.061$
Al ₂ O ₃ (Trigonal)	3.5x10 ⁶ c-axis 3.3x10 ⁶ ⊥ c-axis Reference 15	6.23x10 ⁻⁶ c-axis 5.85x10 ⁻⁶ ⊥ c-axis Reference 16	$s_{11}=s_{22}=2.35 \times 10^{-13}$ $s_{33}=2.17 \times 10^{-13}$ $s_{12}=-.72 \times 10^{-13}$ $s_{23}=s_{13}=-.36 \times 10^{-13}$ $s_{14}=.49 \times 10^{-13}$ $s_{44}=s_{55}=6.94 \times 10^{-13}$ $s_{66}=6.14 \times 10^{-13}$ Reference 14	$c_{11}=c_{22}=4.97 \times 10^{12}$ $c_{33}=4.98 \times 10^{12}$ $c_{12}=1.64 \times 10^{12}$ $c_{23}=c_{13}=1.11 \times 10^{12}$ $c_{14}=-0.24 \times 10^{12}$ $c_{44}=c_{55}=1.47 \times 10^{12}$ $c_{66}=1.67 \times 10^{12}$ Reference 14	$p_{11}=p_{22}=-.25$ $p_{33}=-.23$ $p_{12}=-.04$ $p_{13}=.005$ $p_{31}=-.03$ $p_{14}=.02$ $p_{41}=.01$ $p_{44}=-.1$ Reference 14

Crystal Material	Thermal Conductivity erg/(cm ² K)	Thermal Expansion Ratio (°K) ⁻¹	Elastic Compliances (cm ² /dyne)	Elastic Stiffnesses (dyne/cm ²)	Elasto-Optic Coefficients (Dimensionless)
KH ₂ PO ₄ (Tetragonal)	2.09x10 ⁵ c-axis 1.86x10 ⁵ a-axis Reference 15	4.40x10 ⁻⁵ c-axis 2.49x10 ⁻⁵ a-axis Reference 16	s ₁₁ =s ₂₂ =1.78x10 ⁻¹² s ₁₂ =-3.8x10 ⁻¹³ s ₂₃ =s ₁₃ =0.71x10 ⁻¹³ s ₃₃ =2.03x10 ⁻¹² s ₄₄ =s ₅₅ =8.1x10 ⁻¹² s ₆₆ =1.64x10 ⁻¹¹ Reference 17	c ₁₁ =c ₂₂ =7.14x10 ¹¹ c ₁₂ =-4.9x10 ¹⁰ c ₂₃ =c ₁₃ =1.29x10 ¹¹ c ₃₃ =5.62x10 ¹¹ c ₄₄ =c ₅₅ =1.27x10 ¹¹ c ₆₆ =6.28x10 ¹⁰ Reference 17	No data at this time
SiO ₂ (Hexagonal)	1.05x10 ⁶ c-axis 5.8x10 ⁵ a-axis Reference 15	7.40x10 ⁻⁶ c-axis 1.34x10 ⁻⁵ a-axis Reference 16	s ₁₁ =s ₂₂ =9.41x10 ⁻¹³ s ₁₂ =-6.0x10 ⁻¹⁴ s ₂₃ =s ₁₃ =-2.62x10 ⁻¹³ s ₃₃ =1.06x10 ⁻¹² s ₄₄ =s ₅₅ =2.77x10 ⁻¹² s ₆₆ =2.00x10 ⁻¹² Reference 17	c ₁₁ =c ₂₂ =1.166x10 ¹² c ₁₂ =1.67x10 ¹¹ c ₂₃ =c ₁₃ =3.28x10 ¹¹ c ₃₃ =1.104x10 ¹² c ₄₄ =c ₅₅ =3.61x10 ¹¹ c ₆₆ =5.00x10 ¹¹ Reference 17	No data at this time

Crystal Material	Thermal Conductivity erg/(cm ² *K)	Thermal Expansion Ratio (°K) ⁻¹	Elastic Compliances (cm ² /dyne)	Elastic Stiffnesses (dyne/cm ²)	Elasto-Optic Coefficients (Dimensionless)
CaCO ₃ (Ortho-rhombic)		1.016×10^{-5} a-axis 1.719×10^{-5} b-axis 3.46×10^{-5} c-axis Reference 16	$s_{11} = 6.95 \times 10^{-13}$ $s_{22} = 1.32 \times 10^{-12}$ $s_{33} = 1.22 \times 10^{-12}$ $s_{44} = 2.43 \times 10^{-12}$ $s_{55} = 3.90 \times 10^{-12}$ $s_{66} = 2.34 \times 10^{-12}$ $s_{12} = -3.00 \times 10^{-13}$ $s_{13} = 4.00 \times 10^{-14}$ $s_{23} = -2.4 \times 10^{-13}$ Reference 17	$c_{11} = 1.60 \times 10^{12}$ $c_{22} = 8.5 \times 10^{11}$ $c_{33} = 8.5 \times 10^{11}$ $c_{44} = 4.12 \times 10^{11}$ $c_{55} = 2.56 \times 10^{11}$ $c_{66} = 4.27 \times 10^{11}$ $c_{12} = 3.73 \times 10^{11}$ $c_{13} = 1.7 \times 10^{10}$ $c_{23} = 1.57 \times 10^{11}$ Reference 17	No data at this time