**3-D TECATE/BREW: Thermal, Stress, and Birefringent
Ray-Tracing Codes for Solid-State Laser Design**

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Summary

This report describes the physics, code formulations, and numerics that are used in the TECATE (totally Eulerian code for anisotropic thermo-elasticity) and BREW (birefringent ray-tracing of electromagnetic waves) codes for laser design. These codes resolve thermal, stress, and birefringent optical effects in 3-D stationary solid-state systems. This suite of three constituent codes is a package referred to as LASRPAK.

Introduction

"Everything should be made as simple as possible, but not simpler."

Albert Einstein
(1879-1955)

The development of high average power (HAP) solid state lasers with large, diffraction-limited beams has been persistently limited by coupled thermal and optical physics effects that are difficult, but not impossible, to resolve in practical system designs. These practical difficulties derive from the fact that both the laser slab and the beam phase and polarization are distorted by three-dimensional (3-D) spatial effects when laser pumping and cooling are applied simultaneously in steady (average power) operation. In efforts to approach the ultimate limits of average power, beam quality, and efficiency, combined theoretical and experimental investigations at LLNL in the late 1980's aimed at gaining a more thorough scientific understanding of the critical issues and developing more effective slab laser design methods. The suite of computational physics codes, LASRPAK, was thus developed, experimentally validated, and used to forge high performance laser designs. The LASRPAK codes have also been modified and applied extensively to evaluate beam steering and depolarization in Nova-class lasers, including the Beamlet demonstration laser and possible Nova upgrade lasers, in more recent work.

The physics model formulations, assumptions, and computational methods in the LASRPAK codes are presented in this report. Sample problems that illustrate significant results of the codes abound in other presentations. It has been necessary for tractability to describe only the 3-D steady state code versions for isotropic media. The physical models and numerical methods used in the heat and stress codes (TECATE) are however structured to apply also to anisotropic media and to transient behavior. The ray tracing codes (BREW) for slab optics will require major modifications for anisotropic laser host media. Thermo-optical codes with lower spatial dimensionality (1-D and 2-D) have also been developed and applied during our earlier work, but they are not included in LASRPAK because HAP laser performance factors and beam steering and depolarization effects in Nova-class ultimately require 3-D resolution.

This report is organized to first develop a birefringent optical model for zig-zag slab amplifiers. The heat and material stress/strain/displacement models are then formulated in later sections. The numerical methods that are used to solve the 3-D heat and material deformation equations are summarized briefly in the final section of this report. (Also see References 1 and 2.)

The LASRPAK codes have been in a constant state of change; they have been modified, extended, and restructured for countless investigations by now. Immediacy of applications has so far overshadowed considerations of code maintenance and portability. The present LASRPAK code versions are therefore neither user-proof nor

user-friendly at this time. The codes are described here in the context of high average power laser applications to ensure that some measure of code documentation is completed and not lost in the flurry of pushing onward to new applications in Nova-class lasers.

1. Preliminaries

When a flashlamp-pumped glass laser slab is convectively cooled to sustain average power operation at practical temperatures, the slab surfaces deform; and both temperature and stress gradients are established in the slab volume. When high average power outputs (1–1000 watts) are approached, optical beams that propagate through the slab acquire discernible aberrations from (i) refraction through thermally distorted beam entrance and exit surfaces; (ii) total internal reflections at thermally deformed slab surfaces, (iii) lensing effects from temperature gradients and stresses in the slab; and (v) depolarization from stress gradients. At sufficiently high average power levels, slabs fracture due to the presence of large tensile stresses and materials defects in slab surfaces. Crystalline laser slabs are subject to these same thermal and optical effects, and require additional considerations of a material anisotropy for the various crystal symmetry classes that were included in previous 2-D code versions.

It is well-known that undesired lensing effects occur at relatively low average power levels when a beam is allowed to propagate straight-through a pumped and cooled laser rod or slab. The zig-zag beam configuration shown in Fig. 1 was conceived to eliminate such lensing effects. In the most ideal physical circumstances, where beam paths are straight lines, where opposing slab surfaces are perfectly flat and parallel, and where both temperature and stress isocontours are perfectly flat and parallel, to the large (pumped) slab surfaces, the optical path length (OPL) of every ray in the beam is identical.⁽³⁾⁽⁴⁾ In this case, with a linearly polarized plane wave incident on the slab, both optical path differences (OPDs) and intensity depolarization (DP) are null over the entire slab aperture in the output beam. But such ideal conditions are never realized in practice. The practical objective in the HAPL program was to design lasers with high beam quality (OPDs < one laser wavelength and DP < 0.01) near tensile stress limits. Our approach first determined the deviations from ideal zig-zag conditions that occur with real laser materials in practically attainable operating conditions; we then developed and applied a design methodology that minimizes optical aberrations at high power outputs.

1.1 Optics in Slabs

Wavefront phase distortions are measured by differences in optical path lengths (OPLs) between various rays, where

$$\text{OPL} \equiv \int n \, ds = \int \left(n^0 + \frac{\partial n}{\partial T} dT + \frac{\partial n}{\partial \sigma} d\sigma \right) ds \quad (1)$$

The refractive index in unperturbed media is denoted by n^0 , and both $\partial n / \partial T$ and $\partial n / \partial \sigma$ are material constants. Refractive indices (n) in a pumped and cooled slab are functions of 3-D temperature (T) and stress(s) distributions. Ray path lengths (s) are determined

Slab geometry:

$M = 6 \equiv$ total number of beam bounces on slab TIR surfaces

$HFP = HT \cdot \tan \psi \equiv$ one-half of beam footprint distance on TIR surfaces

$Length = (M+1) HFP \equiv$ tip-to-tip length of slab

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Fig. 1. Schematic representation of an idealized 6-bounce zig-zag slab.

by propagation distances along generally curved trajectories. Since laser slabs are usually mounted in soft elastomeric materials to eliminate mechanical surface stresses, we assume that depolarization of optical fields is caused only by thermal stress variations. Figure 2 shows greatly magnified slab surface deformations that occur in pumped and cooled amplifiers. The large slab surfaces are frequently referred to as TIR (total internal reflection) surfaces in zig-zag beam geometry. The TIR surface deformations in the x-y planar cut of Fig. 2 give rise to OPD isocontour (fringe) variations primarily in the transverse (x) direction. We note that the magnitude of these deformations is multiplied by each beam bounce in their contribution to transverse OPDs. Deformations of TIR surfaces in y-z planar cuts generate OPDs largely from the longitudinal (z) variations that various rays (i, j) sample along their propagation paths. Fringe patterns that characterize these transverse and longitudinal contributions to wavefront aberrations are also shown schematically in Fig. 2. Deformations of the beam entrance and exit surfaces contribute to both transverse and longitudinal OPD variations as do the temperature and stress distributions in real laser systems.

1.2 Birefringent Ray Tracing

When light propagates through isotropic solids under stress, the speed of propagation depends on the direction of propagation and on the polarization of the light. For a given direction of propagation in a stressed solid there are generally two admissible phase velocities, $v_{1,2} = c/n_{1,2}$; these two values are associated with mutually orthogonal components of the electromagnetic displacement field vector D . The speed of light in vacuum is denoted by c , and the refractive indices n_1 and n_2 must be determined locally as a function of stresses in the slab and of the direction of propagation. Since temperatures, stresses, and refractive indices are spatially variable, electromagnetic waves propagate along curved trajectories according to the eikonal equation

$$\frac{d}{da} \left(n \frac{d\mathbf{r}}{da} \right) = \nabla n(\mathbf{r}) \quad (2)$$

where $\mathbf{r}$ is a position vector, and a is the arc length of propagation. We must therefore solve at arbitrary slab co-ordinates (x, y, z) the simultaneous problem of birefringent propagation on curved paths for both beam phase and polarization. This problem, which includes refraction of wavefronts at thermally distorted slab entrance and exit surfaces as well as beam reflections at deformed zig-zag slab TIR surfaces, is intractable by analytic methods; it is therefore modeled by a 3-D ray tracing method in the BREW (birefringent ray-tracing of electromagnetic waves) code. Although the BREW code traces wave normals, we still refer to it as a ray-tracing code for the sake of convenience. Figure 3 shows some significant aspects of the BREW model. Wave normals of incident plane waves are traced between reference planes R_1 and R_2 . The polarizations of the incident and emergent fields are designated in terms of their s and p -components at R_1 and R_2 , respectively. Numerical computations in the slab are executed on a 3-D

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Fig. 2. Zig-zag slab with greatly magnified surface deformations.

Fig. 3. Schematic view of ray tracing calculations in a zig-zag slab (from Fig. 6-68, 1987 Laser Annual).

discretized grid mesh. Mesh elements are referred to as grid cells, and corners of grid cells as grid nodes with co-ordinates (x, y, z) . Slab temperatures, stress tensor components, and surface displacement vectors (with components u, v, w) are obtained at all nodal points from the TECATE code solutions.

Ray tracing computations start with incident rays that are propagated in air from R_1 to the left wedge face of the slab, where they are refracted into the slab. Propagation within the slab is carried out along those contiguous cells sampled by the rays in their zig-zag paths. Double images have not been observed in current applications, so we use the average index of refraction in each grid cell to compute ray trajectories. The average refractive index is obtained from birefringent eigensolutions of the displacement vector D . These calculations are iterated to ensure that the mutually dependent propagation directions and refractive indices are determined self-consistently as the rays propagate along their trajectories through successive grid cells. Path lengths extend to the deformed TIR surface and wedge face coordinates. Phase shifts at reflection points are included according to Fresnel equations.

2. Physics Model for the Polarization State

Considerable economy of effort is achieved by formulating the polarization model in terms of the displacement field $\mathbf{D}$, which is always perpendicular to the unit wave normal $\mathbf{s} = \mathbf{k}/k$. Following the approach developed in Reference 5, by Yariv and Yeh, the E-field wave equation

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{E} \right) + \epsilon \cdot \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0 \quad (3)$$

can be written as

$$\nabla \times (\nabla \times \boldsymbol{\eta} \cdot \mathbf{D}) - \left(\frac{\omega}{c} \right)^2 \mathbf{D} = 0 \quad (4)$$

$$\text{where } \epsilon_0 \mathbf{E} = \mathbf{h} \cdot \mathbf{D} \quad (5)$$

$$\epsilon_0 \int \text{dielectric permittivity of the vacuum} \quad (6)$$

$$\mu \int \text{magnetic permeability (assumed to be isotropic here)} \quad (7)$$

$$w \int \text{angular frequency of electromagnetic waves} \quad (8)$$

and

$$k = n \frac{w}{c} = n k_0 \quad (9)$$

The impermeability tensor $\boldsymbol{\eta}$ is defined by

$$\eta_{ij} \equiv \epsilon_0 (\epsilon^{-1})_{ij} \quad , \quad i, j = 1, 3 \quad (10)$$

where ϵ^{-1} is the inverse of the dielectric tensor ϵ . The orthogonality relationships between important field quantities are summarized in Fig. 4a. The vectors $\mathbf{D}$, $\mathbf{E}$, and $\mathbf{s}$ are coplanar. Energy flows in the direction of the Poynting vector ($\mathbf{S}$) that is generally not colinear with $\mathbf{s}$. The energy density of the electric field in stressed isotropic media and in anisotropic media is given by

$$U_e = \frac{1}{2} \mathbf{E} \cdot \mathbf{D} \quad (11)$$

Surfaces of constant energy density in $\mathbf{D}$ -space define a general ellipsoid that is referred to as the index ellipsoid. The inner ellipse in Fig. 4a is the intersection of the index ellipsoid with a plane normal to $\mathbf{s}$. The major and minor axes of the ellipsoid are orthogonal eigenvectors $\mathbf{D}_1$ and $\mathbf{D}_2$ that correspond to two normal modes of propagation in equation (4). The magnitudes of the ellipsoid axes provide values of the refractive indices n_1 and n_2 .

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Fig. 4a. Orthogonality and index ellipsoid relationships.

To solve this eigenvalue problem for propagation in a slab, we work in a co-ordinate frame (x', y', z') in which $x' = x$, and z' is always equal to s (the (x, y, z) frame is shown in Fig. 3); i.e.; $s = (001)_T$ and $\nabla = s \partial/\partial z'$. Since s is transverse to D , $(s \cdot D) = 0$; and D_3 is thus null. The wave equation (4) can be reduced by applying the vector identity

$$A \times (B \times C) = B (A \cdot C) - C (A \cdot B) \quad (12)$$

with $A = B = s$, and $C = \partial^2/\partial z'^2 (h \cdot D)$.

The reduced wave equation is

$$\frac{\partial^2}{\partial z'^2} \begin{pmatrix} \eta_{11} & \eta_{12} & \eta_{13} \\ \eta_{21} & \eta_{22} & \eta_{23} \\ 0 & 0 & 0 \end{pmatrix} \cdot D = - \left(\frac{\omega}{c} \right)^2 D \quad (13)$$

Since $D_3 = 0$, the reduced wave equation in the local co-ordinate system (x', y', z') reduces to a 2×2 matrix equation,

$$\frac{\partial^2}{\partial z'^2} \bar{D} = - \left(\frac{\omega}{c} \right)^2 \eta_t^{-1} \cdot \bar{D} \quad (14)$$

where η_t is the transverse impermeability tensor

$$\eta_t = \begin{pmatrix} \eta_{11} & \eta_{12} \\ \eta_{21} & \eta_{22} \end{pmatrix} \quad (15)$$

and

$$\bar{D} \equiv \eta_t \begin{pmatrix} D_1 & D_2 \end{pmatrix}^T \quad (16)$$

By defining a 2×2 index matrix N^2 such that $N^2 \cdot \eta_t = 1$, the reduced wave equation (14) is equivalent to the two differential equations:

$$\frac{\partial}{\partial z'} \bar{D} = \pm i \frac{\omega}{c} N \cdot \bar{D} \quad (17)$$

The plus sign in Eq. (17) describes propagation in the direction of $-z'$, and the minus sign describes propagation in the direction of $+z'$. We solve Eq. (17) with the minus sign to describe the evolution of the polarization state that is associated with the refractive index matrix N . Since the values of both η and η_t are known, both the electric field E and the displacement field D can be obtained readily from the solutions $\tilde{D}$, as will be described in the discussion that follows immediately below.

The dielectric impermeability tensor η is frequently denoted by B in the optics literature. In the compact notation used in both thermoelasticity and photoelasticity,

$$\eta = \begin{pmatrix} \eta_{11} & \eta_{12} & \eta_{13} \\ \eta_{21} & \eta_{22} & \eta_{23} \\ \eta_{31} & \eta_{32} & \eta_{33} \end{pmatrix} \rightarrow \begin{pmatrix} \eta_1 & \eta_6 & \eta_5 \\ \eta_6 & \eta_2 & \eta_4 \\ \eta_5 & \eta_4 & \eta_3 \end{pmatrix} \quad (18)$$

and

$$\eta_t = \begin{pmatrix} \eta_1 & \eta_6 \\ \eta_6 & \eta_2 \end{pmatrix} \quad (19)$$

In the absence of perturbations, we take the x' and y' axes in the local co-ordinate system to be axes of normal mode propagation. When stresses are present, η_t can be written as

$$\eta_t = \begin{pmatrix} \frac{1}{n_{0,1}^2} & 0 \\ 0 & \frac{1}{n_{0,2}^2} \end{pmatrix} + \begin{pmatrix} \Delta\eta_1 & \Delta\eta_6 \\ \Delta\eta_6 & \Delta\eta_2 \end{pmatrix} \quad (20)$$

where

$$\Delta\eta_i = (\Pi \cdot \sigma)_i, \quad i = 1, 6 \quad (21)$$

and

$$\Pi_{ij} \equiv \text{piezo-optical coefficients in compact notation, } i, j = 1, 6. \quad (22)$$

The piezo-optical tensor Π is generally a fourth-rank tensor, and its coefficients are material constants. For isotropic materials

$$n_{0,1}=n_{0,2}=n_0 \equiv n^0 + \frac{dn}{dT} (T - T_0) \quad , \quad (23)$$

where n^0 is the refractive index of the unperturbed material at reference temperature T_0 . In compact notation, isotropy also gives

$$\Pi = \begin{pmatrix} \Pi_{11} & \Pi_{12} & \Pi_{12} & 0 & 0 & 0 \\ \Pi_{12} & \Pi_{11} & \Pi_{12} & 0 & 0 & 0 \\ \Pi_{12} & \Pi_{12} & \Pi_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \Pi_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \Pi_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \Pi_{44} \end{pmatrix} \quad (24)$$

and

$$\Pi_{44} = \Pi_{11} - \Pi_{12} \quad . \quad (25)$$

It follows that

$$(\Pi \cdot \sigma)_1 = \Pi_{11} \sigma_1 + \Pi_{12} (\sigma_2 + \sigma_3) \quad (26)$$

$$(\Pi \cdot \sigma)_2 = \Pi_{12} (\sigma_1 + \sigma_3) + \Pi_{11} \sigma_2 \quad (27)$$

$$(\Pi \cdot \sigma)_3 = \Pi_{12} (\sigma_1 + \sigma_2) + \Pi_{11} \sigma_3 \quad (28)$$

$$(\Pi \cdot \sigma)_j = \Pi_{44} \sigma_j \quad , \quad j = 4, 5, 6 \quad . \quad (29)$$

The perturbations $\Delta \eta_i$ are small in practical solid state lasers, and the index matrix $N = \sqrt{(\eta^{-1})}$ can be evaluated approximately.

One finds that

$$N = \begin{pmatrix} n_0 & 0 \\ 0 & n_0 \end{pmatrix} - \frac{n_0^3}{2} \begin{pmatrix} \Delta\eta_1 & \Delta\eta_6 \\ \Delta\eta_6 & \Delta\eta_2 \end{pmatrix} \equiv \begin{pmatrix} a & c \\ c & b \end{pmatrix} \quad (30)$$

The solution of the reduced wave equation (17) can now be found. The field with wavelength λ_0 evolves from $\tilde{D}(0)$ to $\tilde{D}(\Delta z')$ during propagation along a path of length $\Delta z'$ according to

$$\tilde{D}(\Delta z') = \exp\left(-i \frac{2\pi}{\lambda_0} \int_{s=0}^{\Delta z'} N ds\right) \cdot \tilde{D}(0) \quad (31)$$

The matrix N is diagonalized by a similarity transformation:

$$N_d = R^T(q) N R(q) = \begin{pmatrix} n_1 & 0 \\ 0 & n_2 \end{pmatrix} \quad (32)$$

where R is the rotation matrix

$$R = \begin{pmatrix} \cos q & \sin q \\ -\sin q & \cos q \end{pmatrix} \quad (33)$$

and

$$q = \frac{1}{2} \tan^{-1} \frac{2c}{a-b} \quad (34)$$

The rotation matrix R relates a new frame (x'', y'', z') to the old frame (x', y', z') as shown in Fig. 4b. Notice also that Eq. (32) is the correct rule for transforming stresses and other second-rank tensors to a new frame. The matrix elements N defined by Eqs. (21-30) are spatially dependent, so we approximate $\int_{s=0}^{\Delta z'} N ds$ over each grid cell by the path-averaged quantity $\langle N \rangle \Delta z'$, which will be referred to henceforth as

$$N \Delta z' = \begin{pmatrix} a & c \\ c & b \end{pmatrix} \Delta z' \quad (35)$$

where it is understood that the matrix elements a , b , and c are also path-averaged quantities. The determination of the eigenvalues and their proper positions in the index matrix is somewhat tedious and yields the values

Fig. 4b. Schematic view of co-ordinate transformation convention used in propagation calculations.

$$n_1 = \frac{a+b}{2} + \frac{\Delta}{2} \quad (36)$$

$$n_2 = \frac{a+b}{2} - \frac{\Delta}{2} \quad (37)$$

where the discriminant Δ is

$$\Delta \equiv \left[(a-b)^2 + 4c^2 \right]^{1/2} \quad (38)$$

and

$$a = n_0 - n_0^3 (\Pi \cdot \sigma)_1 \quad (39)$$

$$b = n_0 - \frac{n_0^3}{2} (\Pi \cdot \sigma)_2 \quad (40)$$

$$c = -\frac{n_0^3}{2} (\Pi \cdot \sigma)_3 \quad (41)$$

Using the fact that $R^T(q) \cdot R(q) = R(q) \cdot R^T(q) = 1$, Eq. (31) for $\tilde{D}(\Delta z')$ can be written as

$$\tilde{D}(\Delta z') = R^T(q) \cdot R(q) \cdot \left[\exp(-i k_0 \Delta z' N) R(q) \right] \cdot R^T(q) \cdot R(q) \cdot \tilde{D}(0) \quad (42)$$

or

$$\tilde{D}(\Delta z') = R^T(q) \cdot \begin{pmatrix} \exp(-ik_0 \Delta z' n_1) & 0 \\ 0 & (\exp-ik_0 \Delta z' n_2) \end{pmatrix} \cdot R(q) \cdot \tilde{D}(0) \quad (43)$$

which is frequently written in terms of the Jones matrix J at the grid cell about (x', y', z') as

$$\tilde{D}(\Delta z') = J \cdot \tilde{D}(0) \quad (44)$$

The Jones matrix can also be written as

$$J = \exp(-ik_0 n_{\text{avg}} \Delta z') R^T(q) \cdot \begin{pmatrix} \exp(-ik_0 \Delta n \Delta z') & 0 \\ 0 & \exp(ik_0 \Delta n \Delta z') \end{pmatrix} \cdot R(q) \quad (45)$$

where

$$n_{\text{avg}} \equiv \frac{(n_1 + n_2)}{2} = \frac{(a + b)}{2} \quad (46)$$

$$\Delta n \equiv \frac{(n_1 - n_2)}{2} = \frac{\Delta}{2} \quad (47)$$

$$k_0 \equiv \frac{2\pi}{\lambda_0} \quad (48)$$

Let us pause here to recount the thread of logic followed in the BREW code. Although BREW is referred to as a ray trace code, we are in fact tracing wave normals s and the polarization state described by $\tilde{D}$. The displacement field $D = (D_1 \ D_2 \ 0)^T$ is obtained from $\tilde{D}$ as

$$D = \eta_t^{-1} \cdot \tilde{D} \quad (49)$$

The electric field E is then obtained from D according to Eq. (5):

$$E = \frac{1}{\epsilon_0} \eta \cdot D \quad (50)$$

We note that $(E)_3$ is generally non-zero due to non-zero elements η_{31} and η_{32} in the full matrix η .

It is also apparent in Eqs. (49) and (50) that

$$\tilde{D} = \epsilon_0 (E_1 \ E_2)^T \quad (51)$$

Referring to Fig. 3, an incident electromagnetic field is expressed in terms of its s and p plane wave components. A selected number of its wave normals are traced through vacuum from the reference plane R_1 , through the slab, and finally to reference plane R_2 . When the incident wavefront is refracted at the slab entrance surface, double refraction occurs when non-zero stresses are present in the slab. Figure 5 shows that, strictly speaking, two refracted rays are created in the first incremental volume (grid cells) of

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Fig. 5. Wave vectors for double refraction at the boundary of a slab under stress.

the slab at the air-slab interface. When each of these refracted rays propagate into another grid cell with different stress values, each of the wave normals k_1 and k_2 split into two more waves, and so forth as the field propagates through the slab. Such a proliferation of wavefronts in slabs with arbitrary stress distributions can overwhelm existing computer capacities. It is therefore necessary to simplify the birefringent ray tracing in some physically admissible manner. So long as double images are not observed in high average power laser amplifiers, one finds that the fast and slow waves k_1 and k_2 in Fig. 5 propagate in nearly identical directions and at slightly different speeds. We therefore use the average refractive index n_{avg} to determine the paths of wave normals.

The field evolution in an M-bounce zig-zag slab system is segmented for purposes of discussion into logical units referred to as beam traversals. The evolution of each ray (wave-normal) from the reference plane R_1 , through air ($n = 1$), to the slab entrance face is described by

$$\bar{D}(l_1) = D(l_1) = \exp(-ik_0 l_1) D(0) \quad (52)$$

where l_1 is the path length from R_1 to the point of entrance into the slab and $D(0)$ is the displacement field incident at R_1 . Rays are then traced along their first traversal across the slab from the entrance face to their first internal reflection on one of the large, convectively-cooled TIR surfaces (from point i to l in Fig. 3) according to

$$D = J_1 \cdot D(l_1) = \exp(-ik_0 l_1) J_1 \cdot D(0) \quad (53)$$

The Jones matrix J_1 for any ray in its first traversal across the slab is itself an appropriately ordered product of Jones matrices for propagation through a set of contiguous grid cells (see Fig. 3).

If a total of $N(1)$ grid cells lie along the path of a ray during its first traversal, the product matrix J_1 is represented analytically by

$$J_1 = \left\{ \exp \left[-ik_0 \sum_{p=1}^{N(1)} (n_{\text{avg}} \Delta z)_p \right] \right\} \cdot J_{N(1)}^{(1)} \cdot J_{N(1)-1}^{(1)} \cdots J_2^{(1)} \cdot J_1^{(1)} \quad (54)$$

where $J_p^{(1)}$ represents the Jones matrix given by Eq. (45) for propagation through the p^{th} grid cell. We notice that the argument of the exponential term in Eq. (54) contains the OPL of the ray for its entire first traversal; this scalar phase factor is common to both (fast and slow) wave components and does not affect the polarization.

The Jones matrix for the first TIR is denoted by J_1^R and is expressed as

$$J_1^R = \begin{pmatrix} \exp(-i\delta_{p,1}) & 0 \\ 0 & \exp(-i\delta_{s,1}) \end{pmatrix} \quad (55)$$

where $\delta_{p,1}$ and $\delta_{s,1}$ are the phase changes for the s and p polarization components respectively. These phase changes depend upon both the refractive index ratio $n_R \equiv (n_{\text{ambient}}/n_{\text{slab}})$ and the angle of incidence θ_1 of the first TIR bounce. Fresnel's equations for the m^{th} bounce give

$$\tan(\delta_{p,m}/2) = \frac{(\sin^2 \theta_m - n_R^2)^{1/2}}{n_R^2 \cos \theta_m} \quad (56)$$

$$\tan(\delta_{s,m}/2) = \frac{(\sin^2 \theta_m - n_R^2)^{1/2}}{\cos \theta_m} \quad (57)$$

By defining the relative phase difference

$$\delta_{ps,m} \equiv \delta_{p,m} - \delta_{s,m} \quad (58)$$

it follows from Eqs. (56) and (57), that

$$\tan(\delta_{ps,m}/2) = \frac{\cos \theta_m \sqrt{\sin^2 \theta_m - n_R^2}}{\sin^2 \theta_m} \quad (59)$$

The TIR reflection matrix is then

$$\mathbf{J}_m^R = \exp(-\delta_{p,m}) \begin{pmatrix} 1 & 0 \\ 0 & \exp(i\delta_{ps,m}) \end{pmatrix} \quad (60)$$

The first term in Eq. (60) is a scalar phase factor that is common to both wave components in $\tilde{\mathbf{D}}$ and does not affect the polarization. It is apparent in Eqs. (59) and (60) that depolarization in $\mathbf{J}_m^R$ approaches zero when θ_m approaches either the critical angle θ_c or $\pi/2$.

By assembling in proper order the expressions for alternating propagation traversals and internal reflection to describe an M -bounce zig-zag beam, the field evolution can be written for each ray as

$$\tilde{\mathbf{D}} = \exp[-ik_0(l_1 + l_2)] \mathbf{J}_{M+1}^R \cdot \mathbf{J}_M^R \cdot \mathbf{J}_M \cdots \mathbf{J}_2^R \cdot \mathbf{J}_2 \cdot \mathbf{J}_1^R \cdot \mathbf{J}_1 \cdot \mathbf{D}(\tilde{\mathbf{0}}) \quad (61)$$

where l_2 is the path length from the slab exit face to the reference plane R_2 . It is apparent that the term $\exp(-ik_0(l_1 + l_2))$ and other common exponential factors that

we've mentioned affect only beam phase and can thus be ignored in considerations of depolarization.

2.1 Basic Polarization Behavior in Zig-Zag Slabs

Propagation of light through a solid with its variable stresses and temperatures mapped onto a discretized computational grid is tantamount to propagation through a very large train of distinct optical elements. Since the physical properties of such an optical train may not be immediately evident, either intuitively or analytically from inspection of the Jones matrix products in Eq. (61), we examine here the properties of beam power conservation, depolarization as a function of bounce number (M) for special stress distributions, and a compensation method to minimize depolarization.

2.1.1 Power Conservation

Beam intensity I (W/m²) is proportional to $|E|^2$ and can be written as:

$$I \propto |E_1|^2 + |E_2|^2 \propto |\tilde{D}_1|^2 + |\tilde{D}_2|^2, \quad (62)$$

where E_1 , E_2 , $\tilde{D}_1$, and $\tilde{D}_2$ are transverse field components that are related according to Eq. (51). It can be shown generally that the power flow in anisotropic solids, which includes a glass slab under stress, is the sum of the power carried by the field modes. The exit beam intensity from a 2-bounce zig-zag slab is expressed as

$$|E_{\text{out}}|^2 = \mathbf{E}^\dagger \cdot \mathbf{E} = \mathbf{E}(0)^\dagger \cdot \mathbf{J}_1^\dagger \cdot (\mathbf{J}_1^R)^\dagger \cdot \mathbf{J}_2^\dagger \cdot (\mathbf{J}_2^R)^\dagger \cdot \mathbf{J}_2^R \cdot \mathbf{J}_2 \cdot \mathbf{J}_1^R \cdot \mathbf{J}_1 \cdot \mathbf{E}(0), \quad (63)$$

where $\mathbf{E}^\dagger = (\mathbf{E}_1^* \mathbf{E}_2^*)$ is the complex conjugate transpose matrix of $\mathbf{E} = (\mathbf{E}_1 \mathbf{E}_2)^T$. It is apparent from Eq. (60) that the reflection matrices $\mathbf{J}_m^R$ are Hermitian; i.e.,

$$(\mathbf{J}_m^R)^\dagger \cdot \mathbf{J}_m^R = \mathbf{1}. \quad (64)$$

A Jones matrix product $\mathbf{J}_m^\dagger \cdot \mathbf{J}_m$ that spans only two grid cells in a beam traversal is written from Eq. (54) as

$$\mathbf{J}_m^\dagger \cdot \mathbf{J}_m = (\mathbf{J}_1^{(m)})^\dagger \cdot (\mathbf{J}_2^{(m)})^\dagger \cdot \mathbf{J}_2^{(m)} \cdot \mathbf{J}_1^{(m)}. \quad (65)$$

Using Eq. (45), we can evaluate $(\mathbf{J}_2^{(m)})^\dagger \cdot \mathbf{J}_2^{(m)}$ as

$$(\mathbf{J}_2^{(m)})^\dagger \cdot \mathbf{J}_2^{(m)} = \mathbf{R}^T(q_2) \cdot \begin{pmatrix} \exp(i\beta_2) & 0 \\ 0 & \exp(-i\beta_2) \end{pmatrix} \cdot \mathbf{R}(q_2) \cdot \mathbf{R}^T(q_2) \cdot \begin{pmatrix} \exp(-i\beta_2) & 0 \\ 0 & \exp(i\beta_2) \end{pmatrix} \cdot \mathbf{R}(q_2) \quad (66)$$

where

$$\beta_2 \equiv ik_0(\Delta n \Delta z)_2 \quad , \quad (67)$$

$$\mathbf{R}^\dagger = \mathbf{R}^T \quad , \quad (68)$$

and

$$(\mathbf{R}^T)^\dagger = \mathbf{R} \quad . \quad (69)$$

It follows for all grid cells (p) that

$$(\mathbf{J}_p^{(m)})^\dagger \cdot \mathbf{J}_p^{(m)} = 1 \quad (70)$$

and

$$\mathbf{J}_m^\dagger \cdot \mathbf{J}_m = 1 \quad . \quad (71)$$

Using Eqs. (64) and (71) in Eq. (63), we see that

$$|E_{\text{out}}|^2 = |E_1(0)|^2 + |E_2(0)|^2 \quad . \quad (72)$$

and beam intensity is thus conserved in zig-zag slabs.

2.1.2 Depolarization Versus Beam Bounces—Special Cases

2.1.2.1 Null Stresses. In the simplest case of zero stresses, a zig-zag slab behaves like a standard optical rhomb. For example, Fresnel's rhomb⁽⁶⁾ can be constructed as shown in Fig. 6 with $M = 2$, $n_{\text{slab}} = 1.5$, and slab wedge angle = 54° . Linearly polarized light at 45° to the x -axis ($\mathbf{E}(0) = (1 \ 1)^T$) enters at normal incidence. The reflection matrix for each TIR is

$$\mathbf{J}_1^R = \mathbf{J}_2^R = \exp(-i\delta_p) \begin{pmatrix} 1 & 0 \\ 0 & \exp(i\pi/4) \end{pmatrix} \quad . \quad (73)$$

The Jones matrix for each beam traversal is

$$\mathbf{J}_m = \exp(i\phi_m) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad (74)$$

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Fig. 6. Schematic view of Fresnel rhomb ($n_{\text{slab}} = 1.5$). E_{in} is linearly polarized at 45° to x-axis, and E_{out} is circularly polarized.

where the phase factors $\exp i\phi_m$ are functions of optical path lengths in each traversal that are common to each wave component. Polarization is seen here to be unaffected by beam traversals across the unstressed slab. Neglecting all common phase factors, the E -field polarization at slab exit is (from Eqs. (51 and 61))

$$E_{out} \propto J_1^R \cdot J_2^R \cdot E(0) = (1 \ i)^T . \quad (75)$$

It is readily seen⁽⁶⁾ that initial linearly polarized light was transformed to elliptically polarized light after the first TIR and then to circularly polarized light after the second TIR. We therefore anticipate that polarization in zig-zag slabs with non-zero stresses may also be a function of the number (M) of zig-zag beam bounces.

Measures of depolarization are defined from the wave component intensities, $I_s = |E_1|^2$ and $I_p = |E_2|^2$. Depolarization of the initial p - and s - components is expressed by the ratios

$$\Delta P_p = \frac{I_p - I_p(0)}{I_p(0) + I_s(0)} \quad (76)$$

$$\Delta P_s = \frac{I_s - I_s(0)}{I_p(0) + I_s(0)} . \quad (77)$$

When the incident field is entirely s -polarized ($E(0) = (1 \ 0)^T$), we refer to ΔP_p as ΔP_{ps} , which is the fraction of initial s -wave intensity that is observed as emergent p -wave intensity. We define ΔP_{sp} by interchanging p and s in the definition of ΔP . In the present example $I_p(0) = I_s(0) = 1$, and $\Delta P_{ps} = 0$. Although the polarization of the E -field has changed from linear to circular, it is apparent from Eq. (75) that the intensity in the s - and p - components has not been altered by TIR. This result was also evident from the diagonal structure of both the reflection matrices and the Jones matrices for beam traversal in Eqs. (73) and (74).

2.1.2.2 Slabs with 1-D Temperature Distributions. When a 90° zig-zag slab is pumped and cooled uniformly on its TIR surfaces and insulated perfectly on all other smaller (side) surfaces, the resultant temperature isocontours are everywhere perfectly flat and parallel to the TIR surfaces as shown in Fig. 7. Stress isocontours shown in Fig. 7 are similarly 1-D away from side surfaces. But free boundary surfaces cause the stress isocontours to be 3-D near slab edges. In this idealized system, all shear stresses and σ_{yy} are null where the stress contours are 1-D. From here, we show that depolarization DP is null where shear stresses are null. Although this next development is somewhat mathematical in its details, it is worthwhile because it reveals some of the essential physical workings of depolarization (and lack of it) in zig-zag slabs. This development also discusses important aspects of the depolarization model that is computed in the BREW code.

We examine first the field-evolution for the m^{th} beam traversal, i.e.,

$$\tilde{D}_m = J_m \cdot \tilde{D}' , \quad (78)$$

Fig. 7. Schematic view of stress tensor transformations between the laboratory frame (x, y, z) and the beam frame (x', y', z') and of stress eigenvector rotations in the beam frame.

where $\bar{D}'$ is the field-vector just prior to the m th traversal, and J_m is a product Jones matrix of the form shown in Eq. (54). It is most convenient to examine the properties of grid cell Jones matrices in Eq. (45) in terms of real sine and cosine functions; algebraic reductions yield the expression

$$J_p^{(m)} = \exp(-i\phi_p) \left\{ (\cos\beta_p)1 + i \sin\beta_p \begin{pmatrix} -\cos 2q & -\sin 2q \\ -\sin 2q & \cos 2q \end{pmatrix} \right\} \quad (79)$$

where

$$\phi_p \equiv k_0(n_{\text{avg}} \Delta z)_p, \quad (80)$$

and β_p was defined previously in Eq. (67). Equation (79) for $J_p^{(m)}$ can be reduced further by using the relationships that were developed in Eqs. (34) and (38)–(41); we obtain

$$J_p^{(m)} = \exp(-i\phi_p) \left\{ (\cos\beta_p)1 + i \sin\beta_p \begin{pmatrix} -(\sigma'_{22} - \sigma'_{11})/d' & -(\sigma'_{12}/d') \\ -(\sigma'_{12}/d') & (\sigma'_{22} - \sigma'_{11})/d' \end{pmatrix} \right\}, \quad (81)$$

where d' is defined by

$$d' \equiv [(\sigma'_{22} - \sigma'_{11})^2 + (2\sigma'_{12})^2]^{1/2}. \quad (82)$$

Stress values σ'_{ij} in the beam frame (x', y', z') must be obtained by applying the co-ordinate transformation rule for second-rank tensors as ⁽⁷⁾

$$\sigma' = a \cdot \sigma \cdot a^T, \quad (83)$$

where the stresses σ are either measured or computed in the laboratory frame ($x y z$).

For an upward traveling ray shown in Fig. 7, the transformation matrix is

$$a = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & l & -m \\ 0 & m & l \end{pmatrix}, \quad (84)$$

where $l \equiv \cos\psi$

and $m \equiv \sin\psi$.

It can then be shown that σ' is given by

$$\sigma'_{11} = \sigma_{11} \quad (85)$$

$$\sigma'_{12} = \sigma'_{21} = l\sigma_{12} - m\sigma_{13} \quad (86)$$

$$\sigma'_{13} = \sigma'_{31} = l\sigma_{13} + m\sigma_{12} \quad (87)$$

$$\sigma'_{22} = l^2\sigma_{22} - 2lm\sigma_{23} + m^2\sigma_{33} \quad (88)$$

$$\sigma'_{23} = (l^2 - m^2)\sigma_{23} - lm(\sigma_{33} - \sigma_{22}) \quad (89)$$

$$\sigma'_{33} = l^2\sigma_{33} + 2lm\sigma_{23} + m^2\sigma_{22} \quad (90)$$

Values of σ' for downward-traveling waves are obtained by replacing m with $(-m)$ in Eqs. (85-90).

It follows for both upward- and downward-traveling rays that $\sigma'_{12} = 0$, and that

$$J_p^{(m)} = \exp(-i\phi_p) \left\{ (\cos\beta_p)1 + i \sin\beta_p \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right\} \quad (91)$$

in the 1-D stress region in this example. This result has an important consequence:

When all shear stresses are zero, there is no conversion of beam intensity during propagation from one polarization mode to the other; that is,

$$|E_s^{\text{out}}|^2 = |E_s(0)|^2 \quad (92)$$

and

$$|E_p^{\text{out}}|^2 = |E_p(0)|^2 \quad (93)$$

This result was obtained by first applying Eq. (91) in the first grid cell to evaluate

$$E = J_1^{(m)} \cdot \begin{pmatrix} E_1(0) \\ E_2(0) \end{pmatrix} = \begin{pmatrix} C_1 E_1(0) \\ C_1^* E_2(0) \end{pmatrix} \quad (94)$$

where the complex number C_1 is

$$C_1 \equiv \exp(-i\phi_1)(\cos\beta_1 - i\sin\beta_1) \quad (95)$$

Repeated multiplication of Jones matrices $J_p^{(m)}$ preserves the form of the relationship in Eqs. (92)–(94) so that modal intensity conservation holds for the entire beam traversal represented by J_m . Since TIR also does not alter the modal intensity, we find that $\Delta P_{ps} = \Delta P_{sp} = 0$ when all shear stresses are zero and the number (M) of beam bounces is even. It is also evident in this development that non-zero shear stresses are the substantive cause of beam depolarization in zig-zag slabs, as has been confirmed in countless practical and computational examples by now.

2.1.2.3 A Compensation Method for Depolarization in Zig-Zag Slabs. Practical HAP slab laser amplifiers have both pump source variations within their volumes and non-adiabatic thermal conditions on their surfaces. Shear stresses and beam depolarization are therefore inevitable on some portion of the slab output aperture at HAP levels. Recognizing that compensation methods are used to eliminate depolarization in many optical devices, we examine here the limits of applicability of a known compensation method in the thermal environment of HAP laser amplifiers. Figure 8 shows schematically a two-pass compensation method that was suggested for application in our zig-zag slabs by Mark Summers and Bob Boyd.⁽⁸⁾ During the first beam pass through the slab some amount of intensity that was initially in the s -component of the incident beam is transferred (rotated) by birefringence into the p -component of the emergent beam, and vice versa. The central notion of the compensation method is to combine system symmetry and optical operations so that the second pass of the beam exactly retraces the first pass trajectory, with spatial reversal, so as to nullify the field aberrations that were incurred in the first pass. By rotating the beam polarization by 90° between beam passes, the birefringent transfer of intensity that occurred between the p - and s -wave components during the first pass is exactly reversed by propagation in the second pass. The final rotation of -90° after the second pass simply restores the output s - and p -component orientations of the output beam to those of the incident beam. We demonstrate next the physical workings of this method by Jones matrix analysis and then discuss with a computed example means by which practical systems may deviate from the ideal system.

The output field E_{out} for a two-bounce zig-zag slab is expressed as

$$E_{\text{out}} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \underset{\substack{\uparrow \\ \text{Rot}(-90^\circ)}}{J_{\text{rev}}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \underset{\substack{\uparrow \\ \text{Rot}(90^\circ)}}{J_{\text{forward}}} \begin{pmatrix} E_s(0) \\ E_p(0) \end{pmatrix} \quad (96)$$

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Fig. 8. Polarization compensation methods.

The Jones matrices for the forward and reverse beam paths are (from Eq. (61))

$$J_{\text{forward}} = J_1 \cdot J_1^R \cdot J_2 \cdot J_2^R \cdot J_3 \quad (97)$$

$$J_{\text{rev}} = J_3 \cdot J_2^R \cdot J_2 \cdot J_1^R \cdot J_1 \quad (98)$$

We consider without loss of generality the simple case in which each beam traversal of the slab is represented by a single grid cell. It follows from Eq. (45) that

$$J_m = \exp(-i\phi_m) R^T(q_m) \cdot \begin{pmatrix} \exp(-i\beta_m) & 0 \\ 0 & \exp(i\beta_m) \end{pmatrix} \cdot R(q_m) \quad (99)$$

or

$$J_m = \begin{pmatrix} a_m & c_m \\ c_m & b_m \end{pmatrix} \quad m = 1, 3 \quad (100)$$

In order to evaluate Eq. (96) for E_{out} , we consider the matrix product

$$\begin{aligned} J_{\text{prod}} &= J_{\text{rev}} \cdot \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \cdot J_{\text{forward}} \\ &= J_3 \cdot J_2^R \cdot J_2 \cdot J_1^R \cdot J_1 \cdot \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \cdot J_1 \cdot J_1^R \cdot J_2 \cdot J_2^R \cdot J_3 \quad (101) \end{aligned}$$

If J_1 is represented by its matrix $\begin{pmatrix} a_1 & c_1 \\ c_1 & b_1 \end{pmatrix}$, it can be shown in Eq. (101) that

$$J_1 \cdot \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \cdot J_1 = \det(J_1) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (102)$$

It follows from Eq. (102) that the matrix product contracts all the way to the following expression

$$J_{\text{prod}} = S_1 S_2 S_3 S_1^R S_2^R \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (103)$$

where the scalars S_1^R and S_2^R are the determinants of J_1^R and J_2^R , respectively. Substitution of Eqs. (101) and (103) into Eq. (96) yields

$$E_{out} = E(0) \quad , \quad (104)$$

which proves that depolarization is completely conjugated in this ideal two-pass compensation method for zig-zag slabs. The reason this compensation method works arises from the sequence of physical operations that were described in the perfect contraction (conjugation) of Jones matrices for this two-pass system. Other combinations of reflections, rotations, and beam passes can undoubtedly be derived to achieve depolarization compensation in a variety of system architectures; e.g., the two slab and rotator alternative architecture shown in Fig. 8.

Several non-ideal factors can limit the effectiveness of a beam compensation method in a practical laser system. For example, the two slab alternative in Fig. 8 would be practically impossible to maintain at identical operating conditions due to operating tolerances inherent in pump sources in the respective slabs, alone. We do not consider this alternative further at this time. The single slab system in Fig. 8 has been modeled in conjunction with a $1 \times 14 \times 42 \text{ cm}^3$ APG-1 glass slab. The slab wedge angle is 43° and a trial flashlamp pump cavity with a $14 \times 33 \text{ cm}^2$ illumination area on the slab TIR surfaces has been simulated. When pump levels produce peak tensile stresses of 50 MPa, depolarization computed by the BREW code in the uncompensated system was found to be significant ($\Delta P_{ps} \geq 10\%$) over a large portion of beam area. The same slab conditions were computed in the two-pass compensation architecture. The compensation is quite extensive; but it is not completely compensated because the return path of rays in the second pass do not exactly replicate the ray trajectories of the first pass. When different rays emerge from the slab after the first pass, their trajectories are no longer parallel because of their varied sampling of deformed slab surfaces, temperatures gradients, and stress gradients during zig-zag propagation through the slab. Finally, reflection from a perfect mirror between beam passes can also amplify ray path divergences.

3. Thermal Model

An ultimate objective of HAP laser design is to attain beams with minimal phase and polarization aberrations at all power levels short of thermal stress fracture limits. Figure 9 shows schematically a glass zig-zag slab amplifier, which contains several components that are thermo-optically significant. Thermal source functions $Q(x, y, z)$ include heat deposited in: (i) the slab from laser ion pumping, (ii) the elastomer by absorption of pump light, and (iii) the parasitic stopper (ASE cladding) by the absorption of both pump light and amplified spontaneous emission (ASE) photons. Thermal flux boundary conditions on the slab TIR surfaces are determined by properties of the coolant flow and possibly of the evanescent wave coating (EWC) material, as well. Interior thermal fluxes must be continuous at the slab-elastomer interface and at the elastomer-ASE cladding interface. It is assumed that the chill bars maintain a constant temperature at their interface with the ASE cladding. The heat flux at the beam entrance and exit surfaces (wedge faces) are determined by a convective film coefficient for ambient air. In short, the thermal problem is a multiple-region, multiple thermal source problem with simultaneous film and fixed-temperature boundary conditions; it is described by the heat equation

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (\mathbf{k} \cdot \nabla T) + Q(x, y, z) = 0 \quad (105)$$

where

T = temperature ($^{\circ}\text{K}$)

ρ = mass density (kg/m^3)

C_p = heat capacity ($\text{J}/\text{kg} \cdot ^{\circ}\text{K}$)

$\mathbf{k}$ = thermal conductivity tensor ($\text{W}/\text{m} \cdot ^{\circ}\text{K}$)

$Q(x, y, z)$ = rate of internal heat generation | thermal source function (W/m^3).

The thermal conductivity for isotropic solids is a second-rank tensor of simple form

$$\mathbf{k} = \begin{pmatrix} k & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & k \end{pmatrix} = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{pmatrix} \quad (106)$$

The product $-(\mathbf{k} \cdot \nabla T)$ is the heat removal flux $\mathbf{F}$. We assume that thermal conductivities are constant, although this assumption can be relaxed to allow them to be functions of both spatial coordinates and T if necessary at some future time. Convective heat fluxes at slab TIR and wedge surfaces are

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Fig. 9. Zig-zag slab amplifiers are multi-region multi-thermal-source systems.

$$F = -h_c(T - T_{\text{coolant}})n \quad (107)$$

where

h_c is the convective heat transfer, or film, coefficient; and n is the outward unit normal to a slab surface. Continuity of heat fluxes at slab-coolant boundary surfaces is expressed as

$$(k \cdot \nabla T) \cdot n = -h_c(T - T_{\text{coolant}}) \quad (108)$$

Film coefficients h_c assume only positive values and can be functions of spatial coordinates, as can T_{coolant} . *Temperature distributions are therefore determined entirely by the thermal source functions in conjunction with the thermal boundary and interface conditions.*

Average power conditions are taken to be a steady state problem and imply certain temporal assumptions that are depicted in Figure 10. Real pump sources are frequently very short pulses (in time) that are repeated at some pulse repetition frequency (prf). We consider the spatially averaged temperature $\bar{T}_0$ of the slab to be equal to T_0 at time $t = 0$. Each pump pulse thereafter deposits an amount of heat energy $H = \int_{\text{pulse}} dt \int_{\text{slab}} d^3r Q(r, t) = \int_{\text{pulse}} dt H'(t)$ in the slab volume. In response to this heat deposition and to steady thermal boundary conditions on the slab surfaces, $\bar{T}_0$ of the slab will rise in some manner as depicted in Figure 10 during the transient regime. The so-called average power regime is defined somewhat arbitrarily and occurs when transient temperature oscillations from each subsequent pulse have become small relative to $\bar{T}_0$. Average power operation is thus taken to be a sustained condition in which the thermal source function is appropriately time-averaged as shown schematically in Figure 10.

3.1 Slab Thermal Source Function Models

Thermal source functions are the overriding determinants of beam quality. Wavefront aberrations are highly sensitive to the distribution of $Q(x, y, z)$ within the amplifier slab itself and also in contiguous elastomer and/or ASE cladding materials. Three-dimensional thermal source functions are not only difficult to compute accurately, they are extremely difficult, if not impossible, to measure directly within the slab volume. We are therefore faced with using approximated values of $Q(x, y, z)$ in code calculations. In the simplest instances, constant values of Q are used both analytically and in the TECATE (Totally Eulerian Codes for Anisotropic Thermo-Elasticity) codes to illustrate important thermo-optical principles and to validate the codes with problems that have known solutions. In physical reality, flashlamp pump sources are rich in polychromatic detail due to their origin in plasma arcs and to their propagation through intervening lamp coolants, lamp coatings, slab coolants, and the slab itself. Absorption cross sections of doped slabs, elastomers and ASE claddings are spectrally variable over uv, visible and infra-red (IR) wavelengths, which suggests that photons in transparent spectral regions can propagate more or less randomly in the slab and pump cavity until they are eventually absorbed or otherwise lost from the system.

Fig. 10. Average power conditions are defined by time-averaging near thermal steady state.

Photons with wavelengths near spectral line centers may have very short mean free paths. Pump source distributions can thus be quite sensitive to both spectral transport effects and to slab and cavity geometry.

Such ray trace codes as ZAP and MIR3D have been used to resolve this rich array of physical processes with varying levels of success in both pump cavity designs and thermal source evaluations. Our present purposes are served by describing instead an intermediate semi-analytical model of pump source physics that is self-contained in the TECATE code; this model illustrates both energy normalizations and logical relationships between pump absorption, heat energy and power deposition, and observed laser gains that are used in the present codes.

3.2 Semi-Analytical Pump Source Model

When pump photons are absorbed in a slab, heat deposition is inevitable. Figure 11 shows that pump photons excite laser ions to the average pump level at energy $E_p = hc/\lambda_p$. The ions relax non-radiatively to the upper laser level, releasing heat directly into the slab. Additional radiative and non-radiative decays from the upper laser level then proceed either directly or indirectly to the ground state releasing both heat and radiative energy into the slab. We wish to relate the amount of heat deposited in the slab volume to a readily measured physical observable, such as the gain a (m^{-1}). The specific thermal load parameter χ is most frequently used for that purpose. If we consider the energy absorbed (E_{abs}) in the slab volume from a single pump pulse, χ is defined as the ratio of the thermal energy deposited ultimately in the pumped slab to the peak energy stored in the population inversion (or peak stored optical energy) at time $t = \tau_p$, as shown schematically in Figure 12.

The power absorbed in the slab is

$$P_{abs} = E_{abs} f \quad , \quad (109)$$

where f is the pulse frequency. Referring to Figures 11 and 12, one notices that a relationship between P_{abs} and the total peak stored optical energy (ρ_{tot}) in the slab is

$$P_{abs} \cdot QD \cdot d = \int d^3r r_s(r) \cdot f = \rho_{tot} f \quad . \quad (110)$$

where the quantum defect QD is defined by

$$QD = \frac{E_2}{E_p} = \frac{\lambda_p}{\lambda_L} \quad . \quad (111)$$

and the peak-to-total stored energy factor d is shown in Figure 12. The stored optical energy density r_s is related to the laser gain by

$$\rho_s = \phi_{sat} \alpha \quad , \quad (112)$$

Fig. 11. Energy levels of a typical neodymium laser ion in glass or crystal, showing excited ion decay paths and their branching ratios (b_1 - b_4).

Fig. 12. Energy partitioning as a function of time in a doped glass laser slab.

where the saturation fluence f_{sat} is defined by

$$\phi_{sat} = \frac{hc}{\lambda_L \sigma_{emission}} \quad (113)$$

and $\sigma_{emission}$ is the microscopic emission cross section. The term hc is simply the product of Planck's constant (h) and the speed of light (c). The total stored energy in the slab can be expressed in terms of a physically observed gain as

$$\rho_{tot} = \int d^3r \rho_s(r) = \phi_{sat} A_{aperture} \cdot \overline{(\alpha l)} \quad (114)$$

where the slab aperture area is denoted by $A_{aperture}$ and $\overline{(\alpha l)}$ is the aperture-averaged value of gain $\cdot$ length that can be obtained from physical measurement(s).

Thermal source functions $Q(r)$ are computed in the TECATE code from values of ρ_{tot} , χ , and prf that are provided by the user and from a computed spatial distribution function $\tilde{D}(r)$ that is described later in this discussion.* The total thermal power deposited in the glass slab is denoted in the codes as $PWRHTG$, and is the basis of code normalizations; it is defined by

$$PWRHTG \equiv \int d^3r Q(r) = \chi f \rho_{tot} \quad (115)$$

We also define and compute numerically the factor

$$SUMG \equiv \int d^3r \tilde{D}(r) \quad (116)$$

It follows that $Q(r) = (PWRHTG/SUMG)\tilde{D}(r)$.

The power absorbed from pump light in a slab is expressed in terms of the pump absorption rate per unit volume $R_{abs}(r)$ as

$$P_{abs} = \int_{slab} d^3r R_{abs}(r) \quad (W) \quad (117)$$

where

$$R_{abs}(r) = \rho_D \int_{pump\lambda} d\lambda \sigma_{abs}(\lambda) I_{\lambda}(r) \quad (W / m^3) \quad (118)$$

The pump intensity about an arbitrary observation point r in the slab is denoted by $I_{\lambda}(r)$, and $\sigma_{abs}(\lambda)$ is the microscopic cross section for pump light absorption by dopant ions with number density $\rho_D(m^{-3})$. The radiative transfer equation can be solved analytically for the pump intensity in a purely absorbing medium; the solution is expressed as

* The spatial distribution function $\tilde{D}(r)$ is not to be confused with the electromagnetic displacement field $\tilde{D}$ in Section 2.

$$I_{\lambda}(r) = \int_{\text{slab surfaces}} d^3r' \frac{S_{\lambda}(r', r) \exp(-\Sigma_{\lambda}|r'|)}{4\pi|r'|^2} \quad (119)$$

where $S_{\lambda}(r', r)$ is the pump illumination function on slab TIR surfaces at distances r' from r ; and $\Sigma_{\lambda} \equiv \rho_D \sigma_{\text{abs}}(\lambda)$. It is shown in Figure 13 that pump photons can arrive at r from only those source areas that are conically proscribed on the slab TIR surfaces by the critical angle θ_c . The two-color approximation of equation (118) can be written as

$$R_{\text{abs}}(r) = N_1 \int_{\text{slab TIR surfaces}} dr' r'^2 \sin \theta d\theta d\phi A(r', r) \frac{S_0(r')}{|r'|^2} \quad (120)$$

The attenuation factor at r for light sources incident at r' is

$$A(r', r) = B \exp(-Cr') + (1 - B) \exp(-Dr') \quad (121)$$

The coefficients B, C, D have been obtained from the fitting of attenuation that has been measured for a large number of laser glasses⁹, and N_1 is a normalization factor. Given a position vector r in the slab volume and the pump intensity $S_0(r')$ at TIR surfaces, the absorption rate $R_{\text{abs}}(r)$ in Equation (120) is readily evaluated by numerical integration. We then set $N_1 = 1$, and use $\bar{D}(r) = R_{\text{abs}}(r)$ in the TECATE heat code. Spatially variable pump sources $S_0(r')$ can be applied as input in this model, and collimated pump sources (e.g. pump lasers) can be simulated by setting the critical angle $\theta_c \approx 0$.

Recall that the thermal source function $Q(r)$ integrates to the total power value of $\chi \rho_{\text{tot}} f$. The values of ρ_{tot} and f are usually well-known in a practical laser system; but the value of χ can be quite uncertain and problem-specific. Also χ is a transient quantity in principle that is defined at $t = \tau_p$. The most internally consistent values of χ are computed theoretically from rate equations for the heat energy H and ρ_s , as in the GLASSCHI model^{10,11}. Measured quantum efficiencies and excited state relaxation rates are used to model heat deposition in laser glass samples with time-dependent flashlamp radiation pulses¹². These model results have been validated experimentally. It is assumed that all output radiation from the flashlamp passes directly through the slab thickness once, and that all the decay processes can be represented as single-exponential effective lifetime decays. Other assumptions of trapped fluorescence lifetimes (that are dependent upon the slab shape) and of background absorption by impurities or possibly color centers can be supplied as input to the GLASSCHI model by the user. The user of GLASSCHI can also apply a transport factor as a function of wavelength to account for the efficiency of transferring light from the flashlamp to the slab in any specific cavity configuration where such an efficiency factor is known or otherwise estimated. In addition to these spectroscopically-based evaluations of χ , numerous other experimental evaluations of χ have been reported, including: (i) calorimetry and gain measurements in a laser pump/cavity system, (ii) slab fracture morphology in a laser pump/cavity system, and (iii) thermal expansion and gain measurements. Values of χ measured and evaluated for flashlamp-pumped laser glasses by these different experimental methods have typically exhibited variances on

Model Assumption:

Observation point at r is illuminated by point source $S_0(r')$ in conical areas at slab surfaces $Q_{slab}(r) \sim \epsilon \cdot I(r)$

Solves:

$$I(r) \cong \int d\lambda \sigma_{\lambda}^{abs} I_{\lambda}(r) = N_1 \int_{\text{Slab surfaces}} A(r', r) \frac{S_0(r')}{r'^2} r'^2 dr' \sin \theta d\theta d\phi$$

Attenuation factor (from VODEP data)

Required input:

Geometry and VODEP fitting parameters (B, C, D)

Fig. 13. Schematic view of pump absorption model in a purely absorbing medium.

the order of 50%. In some extreme instances such variances have exceeded 100%. Absolute values of thermal energy deposited in slabs are therefore uncertain and require corresponding safety factors to avoid thermal stress fractures in HAP laser designs. TECATE can be used to estimate the total electrical bank power $TPBANK$ that corresponds to a given value of thermal power deposited in the slab. The transfer efficiency factor $TRNSEFF$ is defined as

$$TRNSEFF = PWRHTG/TPBANK. \quad (122)$$

When $TRNSEFF$ is provided as a code input parameter, $TPBANK$ will be printed as part of the diagnostics output. Computed values of $TPBANK$ will, of course, be only as realistic as the values supplied for χ , ρ_{tot} , prf , and $TRNSEFF$. Since system energy balance is not readily expressed in terms of the time-dependent numerator and denominator factors in χ , a data consistency check is included in TECATE code input/output (I/O) as follows: the total pump power absorbed in the slab is eventually distributed to both heat and stored optical energy. From equation (110),

$$P_{abs} = \tau_{tot} f / (QD \cdot d) \quad (123)$$

If Equation (123) is multiplied by unity $= \chi/\chi$, one finds that

$$P_{abs} \cdot 1 = \chi \cdot \rho_{tot} \cdot f / (\chi \cdot QD \cdot \delta) = PWRHIG / (\chi \cdot QD \cdot \delta) \quad (124)$$

If the product $\chi \cdot QD \cdot \delta > 1$, the power distributed to heat alone would exceed the total power absorbed in the slab, which is impossible. Both the quantum defect, (λ_p/λ_L) , and the peak-to-stored energy factor d are usually known quite accurately in HAP laser designs and can be provided as input to the TECATE code. If the product of χ , QD , and δ exceed unity, an output message indicates data inconsistency.

3.3 Other Thermal Sources in HAP Laser Amplifiers

Validations of the TECATE code against experimental testbed data showed that beam quality near slab edges was affected by pump light absorption in the elastomer. It turns out that elastomer absorption can be used constructively to improve beam quality, as indicated by inspection of Figure 14. The entire slab TIR surfaces in Figure 14 are illuminated by a constant fluence of pump light. The pump intensity inside the slab falls off as it nears the pump aperture limits according to geometrical optics considerations. Thermal sources in the elastomer transport heat into that fall-off region and thereby reduce temperature gradients near the slab-edges. The distribution of pump light in the elastomer volume is either variable or null, depending upon problem-specific configurations. Although the transport of pump light in the elastomer is not described analytically in the TECATE heat code, any constant value can be provided for the elastomer thermal source function variable $QEL(W/m^3)$. For example, QEL can be evaluated as

$$Q_{EL} = \rho_{EL} \int_{\text{Elastomer}} d^3r \int_{\text{Pump } \lambda} d\lambda \sigma_{\text{abs}}(\lambda) I_{\lambda}(r) / \int_{\text{Elastomer}} d^3r \quad (125)$$

Absorption cross section data for the elastomer have been measured, and pump intensities $I_{\lambda}(r)$ in the elastomer can be estimated analytically or in cavity design codes. We have thus designed elastomer dimensions more optimally in this way.

Thermal source functions are also found in the parasitic stoppers (Figure 9). These stoppers are designed to absorb fluorescence that emerges from the slab edge surfaces so that it does not return to the slab and deplete upper laser level populations by unwanted stimulated emission modes. Thermal sources due to ASE cladding absorption are evaluated in the TECATE heat code according to the expression

$$Q_{ASE}(x) = \beta I_0 \exp(-\beta x_1) [1 + \exp(-2\beta x_2)] \quad (126)$$

where

$\beta \equiv$ macroscopic absorption coefficient (m^{-1}) for fluorescence in the ASE cladding material;

$I_0 \equiv$ spontaneous emission intensity (W/m^2) at the entrant surface on the ASE cladding;

$x_1 \equiv$ local coordinate for distance from ASE entrant surface to any point x in the cladding;

$x_2 \equiv$ local coordinate for distance from the ASE-chill bar interface (back surface of cladding) to any point x in the cladding. (See Figure 14).

The second exponential term in the square brackets of Equation (126) accounts for absorption of the return flux of ASE that has been reflected from the back side of the ASE cladding. The value of I_0 at the ASE interface is calculated approximately from a simple model in which fluorescence escapes to slab edges as indicated in Figure 15. Fluorescence emitted at the center of the unit sphere can either be lost through the critical angle cones proscribed on the TIR surfaces or reflect around in the slab by TIR, until reaching either edge or wedge surfaces. Fluorescent photons can then escape from the slab or continue to reflect internally. The loss cone area A_c (steradians) on TIR surfaces is

$$A_c = 2(\text{surfaces}) \cdot 2\pi \int_0^{\theta_c} \sin\theta d\theta = 4\pi(1 - \cos\theta_c) \quad (127)$$

The fraction of fluorescent emissions that are lost in A_c is

$$f_L = A_c / 4\pi = 1 - \cos\theta_c \quad (128)$$

Fig. 15. Fluorescence losses are evaluated from a simple geometrical optics model.

But

$$\cos \theta_c = \sqrt{1 - (n_a / n_s)^2} \quad (129)$$

so

$$f_L = 1 - \left[1 - (n_a / n_s)^2 \right]^{1/2} \quad (130)$$

and

$$\cos fac \equiv (1 - f_L) = \cos \theta_c \quad (131)$$

The fluorescent power density emitted at a point is given by

$$P_F(r) = P_{abs}(r) \cdot QD \cdot \tau_D / \tau_R \quad (132)$$

where τ_R is the radiative lifetime of undoped laser slab material, and τ_D is the decay lifetime of doped slab material. If we consider an example of a water-cooled glass slab with dimensions $1 \times 14 \times 40 \text{ cm}^3$ (perimeter = 108 cm) and refractive indices $n_s = 1.53$ and $n_A = 1.33$, it follows that $\cos \theta_c \approx 0.5$ and approximately half ($f_L \approx 0.5$) of the fluorescent photons emitted in the slab are lost through the TIR faces. The ratio of slab edge area to wedge area is approximately 3:1. The fluorescent power that remains in the slab is roughly equal to $P_F(1 - f_L) \approx 0.5P_F$; and the amount that encounters side edge areas is taken to be approximately $\frac{80 \text{ cm}}{108 \text{ cm}} \cdot (.5P_F)$. The fraction of the fluorescence edge fluence that may get absorbed in the ASE cladding is denoted in the TECATE edge heat model as $F5080P \cdot P_F$, where $F5080P$ in this example is $(80/108)(0.5) = .37$. The average fluence of fluorescence at each ASE cladding interface is

$$I_o = F5080P \cdot (P_F / 2) \cdot CLADAR \quad (133)$$

where $CLADAR = 1 \times 40 \text{ cm}^2$ in this example. This simple example has assumed that laser extraction is null, which corresponds to maximum heat loading of the ASE cladding material. Fresnel refraction coefficients are assumed to be 1.0. Direct shine of pump light on the ASE cladding can also be included in the analytic model as an input variable $DIRSHN$. This model is indeed simplistic; it is intended only to represent the essence of physics in the problem. The user can again do much more detailed modeling of edge heating effects to justify values for the parameter $F5080P$.

3.4 Summary of Code Input Data

Thermal code inputs are:

- System geometry and numerical grid designations.
- Thermal source distributions ($Q(x, y, z)$) for all materials/regions; in many cases this input is provided by option flags and values for source function parameters that have been discussed above.
- Boundary condition designations.
 - Dirichlet.
 - Neumann.
 - Film coefficients for convectively cooled surfaces.
- Material data.
 - k for all materials.
 - photon absorption data.
 - radiative lifetimes.
 - data for system energy budget.

4. Thermal Stresses and Material Deformations

The fundamental laws of continuum mechanics describe stresses, strains, and material deformations in simultaneously pumped and cooled solid state laser amplifiers. In practical laser systems numerous simplifications of the fundamental laws are admissible. First, body forces due to gravity and to electric and magnetic sources can be neglected in glass and crystalline HAP laser slabs. Second, mechanical forces on slab exterior surfaces are insignificant because sufficiently soft elastomer materials are used to support a slab in its mounted configuration and because fluid pressure on all cooled surfaces is sufficiently small in systems that we consider. Optical aberrations are then caused only by temperature gradients, thermal stresses, and slab surface deformations in our HAP laser designs. Third, the stress and strain model in the TECATE codes is limited to small elastic deformations because large deformations are optically disastrous and cannot be tolerated in successful thermo-optical designs.

Figure 16 sketches some of the tensor notations and conventions that are used in our thermal stress models. We assume here that the elemental volume in Fig. 16 is a unit cube within the solid, and that its edges are parallel to Ox_1, Ox_2, Ox_3 . Forces are transmitted across each face of the cube by material outside the cube acting upon the material inside the cube. Material stresses σ_{ij} are second-rank tensors; the indices denote the component of physical force in the $+Ox_i$ direction transmitted across the face that is normal to Ox_j . The stress components σ_{11}, σ_{22} , and σ_{33} are referred to as normal components; and $\sigma_{12}, \sigma_{21}, \sigma_{13}, \sigma_{31}, \sigma_{23}$, and σ_{32} are shear components. Positive values of σ_{11}, σ_{22} , and σ_{33} are tensile stresses, and negative values are compressive. When body-torques are absent, which is the case in this work, the stress tensor is symmetric; i.e., $\sigma_{12} = \sigma_{21}$; $\sigma_{13} = \sigma_{31}$; and $\sigma_{23} = \sigma_{32}$. The general equations of thermoelasticity that follow are valid in any event. The indices x, y, z will frequently be used instead of 1, 2, 3, so that $\sigma_{11} \leftrightarrow \sigma_{xx}$; $\sigma_{22} \leftrightarrow \sigma_{yy}$; $\sigma_{33} \leftrightarrow \sigma_{zz}$; $\sigma_{12} \leftrightarrow \sigma_{xy}$; $\sigma_{13} \leftrightarrow \sigma_{xz}$; and $\sigma_{23} \leftrightarrow \sigma_{yz}$. Similarly, we write the material displacement components (u_1, u_2, u_3) as (u, v, w) . The strains for small displacements are defined by

$$e_{ij} = \frac{\partial u_i}{\partial x_j} \quad , \quad i, j = 1, 2, 3 \quad (134)$$

where e_{11}, e_{22} , and e_{33} are the material extensions per unit length parallel to Ox_1, Ox_2 , and Ox_3 ; e_{12} is the rotation about Ox_3 towards Ox_1 of a line element parallel to Ox_2 ; e_{21} is the rotation about Ox_3 towards Ox_2 of a line element parallel to Ox_1 ; etc. The second-rank strain tensor ϵ_{ij} is defined by

$$\epsilon_{ij} = \frac{1}{2} (e_{ij} + e_{ji}) \quad , \quad i, j = 1, 2, 3 \quad (135)$$

and rigid body rotation is defined by the axial vector

$$\omega_{ij} = \frac{1}{2} (e_{ij} - e_{ji}) \quad , \quad i, j = 1, 2, 3 \quad (136)$$

Fig. 16. The forces on the faces of a unit cube in a solid body.

The diagonal elements of the strain $\epsilon_{11}, \epsilon_{22}, \epsilon_{33}$ (or $\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}$), are frequently referred to as tensile strains; and the off-diagonal components $\epsilon_{12}, \epsilon_{13}, \epsilon_{23}$ (or $\epsilon_{xy}, \epsilon_{xz}, \epsilon_{yz}$) are referred to as tensor shear strains. Engineering shear strains $\gamma_{xy} = 2\epsilon_{xy}$, $\gamma_{xz} = 2\epsilon_{xz}$, and $\gamma_{yz} = 2\epsilon_{yz}$ appear frequently in the technical literature and are not to be confused with ϵ_{ij} because γ_{ij} are *not* elements of a tensor and thus do not transform between coordinate frames by tensor transformation rules.

When a material is heated or cooled to some temperature T , relative to a reference temperature T_0 , the resulting contribution to the material strain from temperature alone, is represented by the strain tensor elements,

$$\epsilon_{ij} | \Delta T = \alpha_{ij} (T - T_0) \quad , \quad i, j = 1, 2, 3 \quad (137)$$

where α_{ij} are components of the thermal expansion coefficient α_T . The thermal expansion coefficient is a scalar for isotropic media, and it is generally a function of temperature. We assume that α_T is constant in the present work, although spatial and temperature dependences of α_T can be included in our models, as they are needed.

The continuum model that describes thermal stresses and deformations must be formulated to not only represent the essential physical processes appropriately but to also yield accurate and efficient numerical solutions for the various boundary conditions that may be applied in practical designs. To meet these combined pre-requisites we have developed a coupled set of three partial differential equations (PDE's) that are solved numerically for (u, v, w) in 3-D by a Dynamic Alternating Direction Implicit (DADI) solution method. These equations for (u, v, w) are derived from the balance of force equations ($F = ma$) in the form

$$\nabla \cdot \sigma = 0 \quad , \quad (138)$$

with body forces $ma = 0$. The x -component of this equation is

$$\frac{\partial}{\partial x} \sigma_{xx} + \frac{\partial}{\partial y} \sigma_{xy} + \frac{\partial}{\partial z} \sigma_{zx} = 0 \quad . \quad (139)$$

Hooke's law is used to express stresses in terms of strains and can be written in its general tensor form to describe any solid material as

$$\sigma_{ij} = c_{ijkl} \epsilon_{kl} - \alpha_{ij}(T - T_0) \quad , \quad i, j, k, l = 1, 2, 3 \quad (140)$$

where the c_{ijkl} is a fourth-rank tensor with 81 stiffness constants. Symmetry of the solid reduces the number of non-zero stiffness constants appreciably, as will be seen immediately below for isotropic media.

Symmetry in the first two and the last two suffixes of c_{ijkl} also makes it possible to use a matrix notation that simplifies thermo-elastic analyses. The stress and strain tensor components can be written in terms of a single suffix running from 1 to 6 (also see the textbook by Nye⁷) as:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{31} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{23} & \sigma_{33} \end{bmatrix} \rightarrow \begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{bmatrix} \quad (141)$$

and

$$\begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{31} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix} \rightarrow \begin{bmatrix} \varepsilon_1 & \varepsilon_6/2 & \varepsilon_5/2 \\ \varepsilon_6/2 & \varepsilon_2 & \varepsilon_4/2 \\ \varepsilon_5/2 & \varepsilon_4/2 & \varepsilon_3 \end{bmatrix} \quad (142)$$

In the stiffness matrix c_{ijkl} the first two suffixes are condensed into a single one running from 1 to 6, as are the last two suffixes, according to the following scheme:

tensor notation	11	22	33	23,32	31,13	12,21	
matrix notation	1	2	3	4	5	6	(143)

The array c_{ij} in abbreviated notation is

$$c_{ij} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{bmatrix} \quad (144)$$

The stress equation (140) is then written for isotropic media as

$$\sigma_1 = c_{11} \varepsilon_1 + c_{12} \varepsilon_2 + c_{12} \varepsilon_3 - \bar{\alpha}_T (T - T_0) \quad (145)$$

$$\sigma_2 = c_{12} \varepsilon_1 + c_{11} \varepsilon_2 + c_{12} \varepsilon_3 - \bar{\alpha}_T (T - T_0) \quad (146)$$

$$\sigma_3 = c_{12} \varepsilon_1 + c_{12} \varepsilon_2 + c_{11} \varepsilon_3 - \bar{\alpha}_T (T - T_0) \quad (147)$$

$$\sigma_4 = c_{44} \varepsilon_4 \quad (148)$$

$$\sigma_5 = c_{44} \varepsilon_5 \quad (149)$$

$$\sigma_6 = c_{44} \varepsilon_6 \quad (150)$$

The symmetry properties of isotropic materials are shown diagrammatically by the matrix,

$$c = \begin{bmatrix} \bullet & \bullet & \bullet & \cdot & \cdot & \cdot \\ \cdot & \bullet & \bullet & \cdot & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \times & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \times & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \times \end{bmatrix} \quad (151)$$

The notational key is

$$\begin{array}{ll} \cdot & \text{zero component} \\ \bullet & \text{Non-zero component} \\ \bullet - \bullet & \text{equal components} \\ x & \frac{1}{2} (c_{11} - c_{12}) \end{array}$$

There are only two independent constants in Eqs. (145–150). In terms of the Lamé constants μ and λ , the isotropic stiffness components are

$$c_{11} = 2\mu + \lambda \quad (152)$$

$$c_{12} = \lambda \quad (153)$$

$$c_{44} = \frac{1}{2}(c_{11} - c_{12}) = \mu \quad (154)$$

and the scalar $\bar{\alpha}_T$ is

$$\bar{\alpha}_T = (3\lambda + 2\mu)\alpha_T \quad (155)$$

Lamé's constants for isotropic media can be evaluated in terms of Young's modulus E , Poisson's ratio ν , and the shear modulus G as

$$\mu = \frac{E}{2(1 + \nu)} = G \quad (156)$$

$$\lambda = \frac{E\nu}{(1 + \nu)(1 - 2\nu)} \quad (157)$$

It can also be shown for isotropic media that

$$3\lambda + 2\mu = \frac{E}{1-2\nu} \quad (158)$$

$$2\mu + \lambda = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \quad (159)$$

$$E = \frac{(3\lambda + 2\mu)\mu}{(\lambda + \mu)} \quad (160)$$

and

$$\nu = \frac{\lambda}{2(\mu + \lambda)} \quad (161)$$

By applying the definitions and notations introduced above, Eqs. (145–150) can be written as

$$\sigma_{xx} = (2\mu + \lambda) \epsilon_{xx} + \lambda(\epsilon_{yy} + \epsilon_{zz}) - \bar{\alpha}_T (T - T_0) \quad (162)$$

$$\sigma_{yy} = (2\mu + \lambda) \epsilon_{yy} + \lambda(\epsilon_{xx} + \epsilon_{zz}) - \bar{\alpha}_T (T - T_0) \quad (163)$$

$$\sigma_{zz} = (2\mu + \lambda) \epsilon_{zz} + \lambda(\epsilon_{xx} + \epsilon_{yy}) - \bar{\alpha}_T (T - T_0) \quad (164)$$

$$\sigma_{xy} = 2\mu \epsilon_{xy} \quad (165)$$

$$\sigma_{xz} = 2\mu \epsilon_{xz} \quad (166)$$

$$\sigma_{yz} = 2\mu \epsilon_{yz} \quad (167)$$

By substituting Eqs. (162–167) and

$$\epsilon_{xx} = \frac{\partial u}{\partial x} = u_x \quad (168)$$

$$\epsilon_{yy} = v_y \quad (169)$$

$$\epsilon_{zz} = w_z \quad (170)$$

$$\epsilon_{xy} = \frac{1}{2}(u_y + v_x) \quad (171)$$

$$\epsilon_{xz} = \frac{1}{2} (u_z + w_x) \quad (172)$$

$$\epsilon_{yz} = \frac{1}{2} (v_z + w_y) \quad (173)$$

into Eq. (139), one obtains the first of three coupled PDE's for (u, v, w) :

$$\begin{aligned} & \frac{\partial}{\partial x} \left[(2\mu + \lambda) u_x + \lambda (v_y + w_z) - \bar{\alpha}_T (T - T_0) \right] \\ & + \frac{\partial}{\partial y} \left[\mu (u_y + v_x) \right] + \frac{\partial}{\partial z} \left[\mu (u_z + w_x) \right] = 0 \end{aligned} \quad (174)$$

Similarly, the y-component of Eq. (138) gives the second PDE:

$$\begin{aligned} & \frac{\partial}{\partial x} \left[\mu (u_y + v_x) \right] + \frac{\partial}{\partial y} \left[(2\mu + \lambda) v_y + \lambda (u_x + w_z) - \bar{\alpha}_T (T - T_0) \right] \\ & + \frac{\partial}{\partial z} \left[\mu (v_z + w_y) \right] = 0 \end{aligned} \quad (175)$$

and the z-component of Eq. (138) yields the third PDE:

$$\begin{aligned} & \frac{\partial}{\partial x} \left[\mu (u_z + w_x) \right] + \frac{\partial}{\partial y} \left[\mu (v_z + w_y) \right] + \\ & \frac{\partial}{\partial z} \left[(2\mu + \lambda) w_z + \lambda (u_x + v_y) - \bar{\alpha}_T (T - T_0) \right] = 0 \end{aligned} \quad (176)$$

Rather than gather terms in Eqs. (174-176), the forms written above show clearly that the balance of force Eq. (138) is being solved for (u, v, w) . The forms written above also admit to effective numerical discretizations and to cell loading of matrices in DADI solutions for both interior regions and boundaries. This approach is especially well-suited to multiregion problems that may be addressed in the future. Such problems require that displacements (u, v, w) are single-valued and that $\sigma \cdot n$ is continuous at material interfaces, while $\mu(E, \nu)$ and $\lambda(E, \nu)$ may be discontinuous at such interfaces. Stresses are then computed in the TECATE code by numerically differentiating the solutions (u, v, w) to obtain ϵ , and by using Eqs. (162-167) to evaluate σ . The present TECATE code version evaluates material stresses and displacements only in the amplifier slab. Boundary conditions in the TECATE code include:

- Free surfaces; i.e., $\sigma \cdot \mathbf{n} = 0$, where $\mathbf{n}$ is the outer surface unit normal.
- Static forces on slab surfaces; i.e., $\sigma \cdot \mathbf{n} = p(x,y,z)$.
- Fixed surfaces; i.e., Dirichlet conditions on (u,v,w) .

Stress code inputs are:

- $T(x, y, z)$ from heat code results.
- Slab dimensions and numerical grid geometry.
- Material constants α_T, E, ν .
- Reference temperature T_0 .
- Boundary condition designations.

5. Numerics

The Dynamic Alternating Direction Implicit (DADI) method was extended to three spatial dimensions (3-D) (for the first time here, so far as we know) in order to solve the stationary heat and stress equations for isotropic media in the 3-D TECATE code. This was a direct extension by Said Doss of the numerical methods that we had used previously in the 2-D TECATE code for anisotropic media.^{13,14} We summarize here the reduction to practice of the DADI method to solve the stationary heat equation for zig-zag slabs. The 3-dimensional problem is described by Eqs. (105) and (106) on the domain Ω by

$$k_{11} \frac{\partial^2 T}{\partial x^2} + k_{22} \frac{\partial^2 T}{\partial y^2} + k_{33} \frac{\partial^2 T}{\partial z^2} + 2 \left(k_{12} \frac{\partial^2 T}{\partial x \partial y} + k_{13} \frac{\partial^2 T}{\partial x \partial z} + k_{23} \frac{\partial^2 T}{\partial y \partial z} \right) = -Q \quad (177)$$

The temperature on the boundary $\partial\Omega$ may satisfy both Dirichlet (T is a given function on some subset $\partial\Omega_1$ of $\partial\Omega$) and Neumann (including film) conditions where

(i) Natural Neumann condition: $(\mathbf{k} \cdot \nabla T) \cdot \mathbf{v} = -\mu$ on some subset $\partial\Omega_2$ of $\partial\Omega$, where $\mathbf{v}$ is the outward unit normal to $\partial\Omega_2$, and μ is nonnegative.

(ii) Film condition: $(\mathbf{k} \cdot \nabla T) \cdot \mathbf{v} = -\lambda(T - T_0)$ on $\partial\Omega_3 (= \partial\Omega - \partial\Omega_1 - \partial\Omega_2)$, where T_0 is the coolant or ambient air temperature, depending on the boundary surface being considered. The film coefficient λ assumes only positive values.

A grid mesh that is congruent to zig-zag slab boundaries is defined on Ω and transformed onto a rectangular domain Γ as shown in Fig. 17 according to the following relationships

$$\xi = x \quad (178)$$

$$\eta = y \quad (179)$$

$$\zeta = z - y \cot \alpha \quad (180)$$

It follows (by chain rule differentiation) that

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi} \quad (181)$$

$$\frac{\partial}{\partial y} = \frac{\partial}{\partial \eta} - \cot \alpha \frac{\partial}{\partial \zeta} \quad (182)$$

$\hat{\mathbf{v}}$ and $\hat{\mathbf{n}}$ are the outward unit normals to $\partial\Omega$ and $\partial\Gamma$ respectively

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Fig. 17. The grid mesh that is congruent to the slab boundaries on Ω is transformed onto a rectangular domain Γ for numerical solution of heat and displacement equations.

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial \zeta} \quad (183)$$

$$K_{200} \frac{\partial^2 T}{\partial \xi^2} + K_{020} \frac{\partial^2 T}{\partial \eta^2} + 2K_{011} \frac{\partial^2 T}{\partial \eta \partial \zeta} + K_{002} \frac{\partial^2 T}{\partial \zeta^2} = -Q \quad (184)$$

where for isotropic media

$$K_{200} = k_{11} = k \quad (185)$$

$$K_{020} = k_{22} = k_{11} = k \quad (186)$$

$$K_{002} = k_{33} + (\cot^2 \alpha) k_{22} = k (1 + \cot^2 \alpha) \quad (187)$$

$$K_{011} = -(\cot \alpha) k_{22} = -k \cot \alpha \quad (188)$$

The directional derivative $(K \cdot \nabla T) \cdot \mathbf{v}$ in both Neumann and film boundary conditions on Ω transforms to $\sin \alpha (K \cdot \nabla' T) \cdot \boldsymbol{\eta}$ on the wedge face boundaries and to $(K \cdot \nabla' T) \cdot \boldsymbol{\eta}$ on the other slab boundaries, where $\boldsymbol{\eta}$ is the outward unit normal to $\partial \Gamma$, and $\nabla' = (\partial/\partial \eta, \partial/\partial \xi, \partial/\partial \zeta)$.

5.1 Cell Discretization

The heat equation is discretized for solution by the DADI method on the grid of rectangular parallelopipeds on Γ (Fig. 17). There are n_ξ , n_η and n_ζ numerical grid points in the ξ , η , and ζ directions, respectively. The grid cell intervals may be either uniform or non-uniform in any or all directions. Each grid node P at the intersection of the i^{th} , j^{th} and k^{th} rows and columns is denoted by $P(i, j, k)$. An interior node is surrounded by eight neighboring cells and 27 neighboring grid nodes (including the interior node itself) that lie completely within the parallelopiped Γ . There are three types of boundary nodes: (i) surface nodes are surrounded by four neighboring cells and 18 neighboring grid nodes; (ii) edge nodes are surrounded by two neighboring cells and 12 neighboring grid nodes; and (iii) corner nodes are surrounded by one neighboring cell and 8 neighboring grid nodes. The requisite operator matrices for numerical solution of the heat equation can be written either in terms of conventional center-difference equations as shown in our previous work in 2-D⁽¹⁴⁾ or by using a cell method that is analogous to a method used frequently with finite elements to load the heat equation matrix.

The cell method is used in our present work because it offers great economy of effort, especially at boundaries, in 3-D finite difference discretizations, just as it does in finite element implementations. For example, the second-order term $KT_{\xi\xi}$ in Eq. (184) at

$P(i, j, k)$ is discretized as follows:

1. Consider a line $\vec{O}(P)$ through $P(i, j, k)$ parallel to ξ in Figure 18.
2. Integrate $KT_{\xi\xi}$ on the interval $i-1/2$ to $i+1/2$ on the volume with end areas $[A(\alpha) + A(\beta) + A(\gamma) + A(\delta)]$ normal to $\vec{O}(P)$;

$$I(kT_{\xi\xi}) = \int_{i-1/2}^{i+1/2} kT_{\xi\xi} d\xi d\eta d\zeta = \left(k_{i+1/2} T_{\xi}^{i+1/2} - k_{i-1/2} T_{\xi}^{i-1/2} \right) (A(\alpha) + A(\beta) + A(\gamma) + A(\delta)) \quad (189)$$

3. Approximate $I(kT_{\xi\xi})$ as

$$I(kT_{\xi\xi}) \equiv \left\{ k_{i+1/2} \frac{T_{i+1} - T_i}{\Delta\xi_i} - k_{i-1/2} \frac{T_i - T_{i-1}}{\Delta\xi_{i-1}} \right\} [A(\alpha) + A(\beta) + A(\gamma) + A(\delta)] \quad (190)$$

and note that this expression is valid at material interfaces, as well as at slab interior points.

4. For cell-wise loading of the discretized residual R that is used in DADI solutions of the heat equation, we wish to decompose the terms in Eqs. (189) and (190) into groups that are associated with a single grid cell. We can then run a do-loop over grid cells, rather than over grid nodes; and for each cell in the loop R is loaded with terms of $I(kT_{\xi\xi})$ for all eight grid nodes on that cell. In this way, the elements of R at an interior node $P(i, j, k)$ receive contributions from the eight cells 1, 2, ..., 8 that are shown in Fig. 18.

5. Using cell 1 (denoted by circled -1 in Figure 18) as an example, we load the term $-k_{i-1/2} \frac{T_i - T_{i-1}}{\Delta\xi_{i-1}} A(\alpha)$ from Eq. 190 to $P(i, j, k)$ in R and note that

$$A(\alpha) = \frac{1}{4} A(abph) \quad (191)$$

Similarly the term $+k_{i-1/2} \frac{T_i - T_{i-1}}{\Delta\xi_{i-1}} A(\alpha)$ from Eq. (190) loads into R at $P(i-1, j, k)$, and so forth for all the nodes on cell 1. By the time all of the terms from cells 1, 2, ..., 8, have been loaded into R , the entire operator $I(kT_{\xi\xi})$ at $P(i, j, k)$ has been loaded properly.

6. When loading is completed for all cells in the problem, the elements of R at each node $P(i, j, k)$ are divided by the cell volume

Fig. 18. Schematic representation of 3-D grid used in cell-loading procedures for PDE discretizations.

$$V = \frac{(\Delta\xi_i + \Delta\xi_{i-1})}{2} \frac{A(P)}{4} \quad (192)$$

where

$$\frac{A(P)}{4} = A(\alpha) + A(\beta) + A(\gamma) + A(\delta) = \frac{A(aceg)}{4} \quad (193)$$

at $\xi = \xi_i$.

7. Cell-loading runs over all grid cells in the problem and is identical for all grid cells.

8. Some operators may require the loading of additional terms into R. Consider, for example, the end faces of cells 1, 2, 3, 4 to be a boundary surface at $\xi = \xi_{i-1}$. In cell 1, the cell-loading procedure at $P(i-1, j, k)$ has loaded $I(kT_{\xi\xi})$ from only one side (the inside) into R. For a film boundary condition, the "outside" portion of $I(kT_{\xi\xi}) = -\lambda(T_{i-1} - T_0)$ $A(\alpha) \cdot n$ must be added to R at $P(i-1, j, k)$. Of course, for Dirichlet boundary conditions no additional terms are required in R. It can also be shown that such terms $T_{\eta\eta}$, $T_{\zeta\zeta}$, and cross-derivatives require no additional terms to be loaded into R at this boundary face.

9. The loading procedures for other operators in Eq. (184) and for other boundary surfaces follow the same principles that were described in this example.

5.2 Solution of The 3-D Heat Equation by Dynamic ADI (DADI)

The discretized heat equation can be written as

$$Lu = f \quad (194)$$

where L is a linear elliptic operator. By writing $L = A + B + C$, and converting Eq. (194) to an evolution equation, we solve

$$\frac{\partial v}{\partial t} = Av + Bv + Cv - f \quad ; \quad t > 0 \quad (195)$$

where the operator A is not to be confused with the area $A(\alpha)$, and v = some initial estimate u^0 at $t = 0$, whose steady state solution ($t \rightarrow \infty$) is a solution of Eq. (194). In order to solve the heat equation, Eqns. (194) and (195) are written as

$$Au = kT_{\xi\xi} \quad (196)$$

$$Bu = kT_{\eta\eta} \quad (197)$$

$$Cu = kT_{\zeta\zeta} \quad (198)$$

$$f = -Q - 2kT_{\eta\zeta} \quad (199)$$

The DADI method solves Eq. (195) by a series of iterative steps (or sweeps) in alternative spatial directions. On the first sweep (ξ - sweep) at the time t_n we solve

$$\frac{u^* - u^n}{\Delta t} = Au^* + Bu^n + Cu^n - f \quad (200)$$

By writing $\delta u^* \equiv u^* - u^n$,

$$\left(\frac{1}{\Delta t} - A\right)\delta u^* = Au^n + Bu^n + Cu^n - f \equiv \text{Residual at } u^n \quad (201)$$

The matrices A, B, and C are easily inverted, so the major computational effort is associated with the loading and evaluation of the partial differential equation residual. The η - sweep solves

$$\left(\frac{1}{\Delta t} - B\right)\delta u^{**} = Au^* + Bu^n + Cu^n - f \equiv \frac{\delta u^*}{\Delta t} \text{ (from Eqn. 200)} \quad (202)$$

Finally the ζ - sweep gives

$$\frac{u^{n+1} - u^n}{\Delta t} = Au^* + Bu^{**} + Cu^{n+1} - f, \quad (203a)$$

or

$$\left(\frac{1}{\Delta t} - C\right)\delta u = Au^* + Bu^{**} + Cu^n - f \equiv \frac{\delta u^{**}}{\Delta t} \text{ (from Eqn. 202)} \quad (203b)$$

The solution u^{n+1} is the $(n + 1)^{\text{st}}$ iterative solution. This 3-D DADI method uses the test parameter strategy for the selection of optimal Δt 's that we used in our previous 2-D work.⁽¹⁴⁾ This strategy changes Δt dynamically in order to: (1) keep Δt within regions of fast convergence, (2) recognize and suppress instabilities by decreasing Δt as they

start to grow, and (3) attain greater efficiency in the choice of iteration parameters than is achieved in the standard ADI method.

Figure 19 sketches this DADI solution strategy schematically. Extensive analysis has shown that this method yields numerical solutions that are accurate to within local truncation errors proportional to h^2 where h is the spatial grid cell dimension.

An ADI step is one triple sweep of ξ , η , and ζ .

$$TP \equiv \text{Test Parameter} = \frac{\|v^{n+2} - \tilde{v}^{n+2}\|}{\|v^{n+2} - v^n\|} = \frac{\|e^{n+2} - \tilde{e}^{n+2}\|}{\|e^{n+2} - e^n\|}$$

where the error $e^n = v - v^n$, and v is the exact solution.

Δt is selected dynamically to maintain $0.1 \leq TP \leq 0.3$ for rapid convergence to steady state solution

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Fig. 19. The DADI test parameter strategy yields unconditionally stable solutions of the heat equation.

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Appendix

We present here two test examples that were solved by the 3-D DADI solution method in the TECATE code.

A test example with a polynomial solution was formulated and solved for one validation of the 3-D DADI method

Given: Heat equation solution $T(x, y, z) = \sum_{i,j,k=0}^4 x^i y^j z^k$

Construct: Test problem with source function $Q = -k\nabla^2 T(x, y, z)$, $k = 1.0$, and with Dirichlet boundary conditions on a $1.0 \times 0.5 \times 2.0 \text{ cm}^3$ rectangular slab

Results:

- Isocontours of relative error $|T - T_{\text{exact}}|_{\text{max}} / |T_{\text{exact}}|$ are plotted in attached figure
- Maximum relative error = 2.98×10^{-5} , as shown in attached figure
- Exact numerical solutions are obtained for polynomials with
 $i, j, k \leq 3$ on uniform grid mesh
 $i, j, k \leq 2$ on non-uniform grid mesh

Isocontours of relative error in 3-D DADI solution of polynomial test problem are plotted at mid-planes of $1.0 \times 0.5 \times 2.0 \text{ cm}^3$ slab

A flashlamp-pumped, convectively-cooled glass zig-zag slab laser example was solved with 3-D DADI method in TECATE code

Thermal conductivity	Glass	Elastomer	ASE absorber
$k \text{ (W/m}^\circ\text{C)}$	1.03	0.19	0.88

Film heat transfer coefficients: $\lambda \text{ (W/m}^2 \text{ }^\circ\text{C)} = 1.5 \times 10^4 \text{ (H}_2\text{O)}$ and $\lambda = 10 \text{ (air)}$

Glass slab dimensions: Length = 32 cm; Width = 10 cm; Ht = 1.5 cm; $\alpha = 28^\circ$

Pump area = $10 \times 20 \text{ cm}^2$ top and bottom

Total power absorbed in slab as heat = 100 W

3-D DADI temperature isocontours are plotted at three midplanes of pumped laser slab

ADI steps = 51
CPU seconds = 30
Convergence tolerance = 10^{-6}