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Algorithm for solutions of the thermal diffusion equation in a stratified medium with a modulated heating source

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Abstract. Thermal diffusion in stratified media is important in many applications such as electronic packaging, optical disk recording, and nondestructive evaluation. A straightforward 'back of the envelope' algorithm is presented for solving the one-dimensional thermal diffusion equation in a stratified medium containing a modulated heating source located at an arbitrary point; interface thermal resistance is easily incorporated. This solution is the Green function for computing the temperature distribution due to a distributed heat source. The solution for the surface temperature of a delaminated film on a substrate is presented as an example of the utility of the method.

1 Introduction

The solutions of the thermal diffusion equation in a stratified (multilayer) medium are important for many modern applications such as thermal diffusivity measurements (Reichling and Grönbeck 1994), thermal wave nondestructive probes (Spicer et al 1993; Feldman 1997), heat conduction in optical disk recording (Shih 1995), and heat dissipation in electronic multilayer structures (Albers 1995). Several analyses have been made of AC or DC steady-state heat flow in general multilayer systems (Carslaw and Jaeger 1959; Kusuda 1969; Kokkas 1974; Aamodt and Murphy 1986; Albers 1995).

The purpose of this paper is to present a simple and versatile algorithm to solve the one-dimensional heat diffusion equation for a general multilayer stack containing a modulated (AC) heating source located at an arbitrary plane within the stack. The algorithm involves a matrix formalism that is analogous to that given previously (Carslaw and Jaeger 1959); thermal resistance at each interface is easily incorporated into the solution. Whereas most previous matrix formalisms have used temperature and heat flux as vector components, this treatment chooses the vector components to be counter-propagating thermal waves; it is analogous to the matrix treatment of light propagation in interference filters (Born and Wolf 1965). The procedure has been used successfully in modeling the thermal signal resulting from the delamination of a diamond film on a tungsten carbide substrate (Feldman 1997). In the case of a distributed heat source, the procedure given here gives the Green function that can be used in obtaining the temperature distribution.

Recently, several authors have treated the propagation of thermal waves in linearly inhomogeneous materials (Fivez and Thoen 1994, 1996) with the thermal conductivity (diffusivity) gradient normal to the specimen surfaces. The procedure presented here can treat any continuous profile as a series of uniform layers; however, it is most convenient for discrete layers.

2 Matrix formulation

The one-dimensional homogeneous differential equation that describes steady-state heat diffusion due to a modulated heat source of angular frequency ω is:

$$\frac{\mathrm{d}^2 T}{\mathrm{d}z^2} + \mathrm{i}\frac{\omega}{D} T = 0 \ , \tag{1}$$

where D is the thermal diffusivity and T is the complex temperature at ω. The time dependent heat source is $q\exp(-\mathrm{i}\omega t)$, where t is time. We assume that D for any single medium is homogeneous, isotropic, and independent of T. The heat source has not been included in the equation as is usually done; instead, heating is treated as a boundary condition which considerably simplifies the solution of the equation. The solution for the temperature distribution in a medium j can be written as the sum of exponential terms representing thermal waves traveling in the $+z$ and $-z$ directions:

$$T(z) = T_j^+\exp(u_j z) + T_j^-\exp(-u_j z) \;, \tag{2}$$

where $u_j^2 = -\mathrm{i}(\omega/D_j)$, and T_j^+ and T_j^- are complex constants to be determined. The temperature can be treated as a two-dimensional vector, $\boldsymbol{T}$, given by:

$$\boldsymbol{T} = \begin{bmatrix} T_j^+(z) \\ T_j^-(z) \end{bmatrix} \;, \tag{3}$$

where each vector component corresponds to a term in equation (2).

Consider a boundary plane at $z = \xi$ between media a and b, as seen in figure 1, with a heat source, q, in the vicinity of the boundary. The temperature and heat flow are continuous across the boundary, thus:

$$T_\mathrm{a}(\xi^-) = T_\mathrm{b}(\xi^+) \;, \tag{4}$$

$$\kappa_\mathrm{a}\frac{\mathrm{d}T_\mathrm{a}}{\mathrm{d}z}\bigg|_{z=\xi^-} = \kappa_\mathrm{b}\frac{\mathrm{d}T_\mathrm{b}}{\mathrm{d}z}\bigg|_{z=\xi^+} + q \;, \tag{5}$$

where ξ^+ is the limit as z approaches the boundary from the right, ξ^- is the limit as z approaches the boundary from the left, and κ_j is the thermal conductivity of medium j. The thermal conductivity is related to the thermal diffusivity by $\kappa_j = D_j\rho_j C_j$, where ρ_j is the mass density and C_j is the specific heat. Using equations (2), (4), and (5), we can obtain several relationships between the temperatures at different points in the material. These relationships are:

(i) The temperature at z_j in medium a in terms of the temperature at z_i in medium a; no intervening heat source.

$$\boldsymbol{T}_\mathrm{a}(z_j) = \mathbf{U}_\mathrm{a}(L)\boldsymbol{T}_\mathrm{a}(z_i) \;, \tag{6}$$

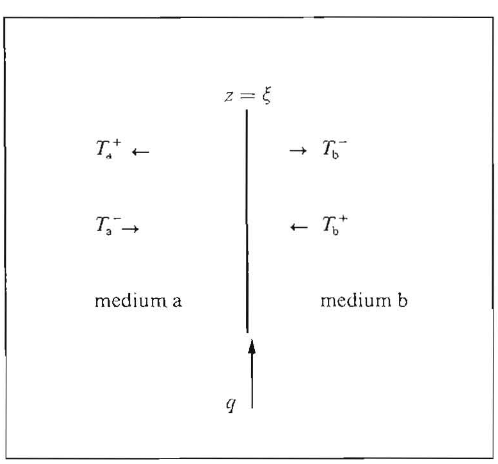

Figure 1. Heating at a boundary between two media.

where

$$\mathbf{U}_{\mathrm{a}}(L) = \begin{bmatrix} \exp(u_{\mathrm{a}}L) & 0 \\ 0 & \exp(-u_{\mathrm{a}}L) \end{bmatrix} , \tag{7}$$

and $L = z_j - z_i$.

(ii) The temperature at a point in medium b adjacent to the boundary between medium a and medium b in terms of the temperature at a point in medium a adjacent to the boundary; no intervening heat source.

$$\boldsymbol{T}_{\mathrm{b}} = \boldsymbol{\Gamma}_{\mathrm{ba}} \boldsymbol{T}_{\mathrm{a}} , \tag{8}$$

where

$$\boldsymbol{\Gamma}_{\mathrm{ba}} = \frac{1}{2\gamma_{\mathrm{b}}} \begin{pmatrix} \gamma_{\mathrm{b}} + \gamma_{\mathrm{a}} & \gamma_{\mathrm{b}} - \gamma_{\mathrm{a}} \\ \gamma_{\mathrm{b}} - \gamma_{\mathrm{a}} & \gamma_{\mathrm{b}} + \gamma_{\mathrm{a}} \end{pmatrix} , \tag{9}$$

and $\gamma_j = u_j \kappa_j$.

If there is a thermal resistance, R_{ab} (Carslaw and Jaeger 1959) at the boundary between medium a and medium b, then the expression to use for $\boldsymbol{\Gamma}_{\mathrm{ba}}$ is:

$$\boldsymbol{\Gamma}_{\mathrm{ba}} = \frac{1}{2\gamma_{\mathrm{b}}} \begin{pmatrix} \gamma_{\mathrm{b}} + \gamma_{\mathrm{a}} + \gamma_{\mathrm{b}}\gamma_{\mathrm{a}}R_{\mathrm{ab}} & \gamma_{\mathrm{b}} - \gamma_{\mathrm{a}} - \gamma_{\mathrm{b}}\gamma_{\mathrm{a}}R_{\mathrm{ab}} \\ \gamma_{\mathrm{b}} - \gamma_{\mathrm{a}} + \gamma_{\mathrm{b}}\gamma_{\mathrm{a}}R_{\mathrm{ab}} & \gamma_{\mathrm{b}} + \gamma_{\mathrm{a}} - \gamma_{\mathrm{b}}\gamma_{\mathrm{a}}R_{\mathrm{ab}} \end{pmatrix} . \tag{10}$$

Note that $R_{\mathrm{ab}} = -R_{\mathrm{ba}}$.

(iii) The temperature at a point adjacent to one side of a heat source located in medium a at position $z = \xi$ to the temperature at a point in medium a adjacent to the other side of the heat source.

$$\boldsymbol{T}_{\mathrm{a}}(\xi^{+}) - \boldsymbol{T}_{\mathrm{a}}(\xi^{-}) = -\frac{q}{2\gamma_{\mathrm{a}}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} . \tag{11}$$

Heating at a boundary between two different media can be considered as heating within one of the media in the limit that the distance between the heat source and the boundary is vanishingly small.

3 General procedure

Consider a multilayer system as seen in figure 2. Using the matrix relationships described above, we want to solve for the temperature at every point for heat input at any particular point.

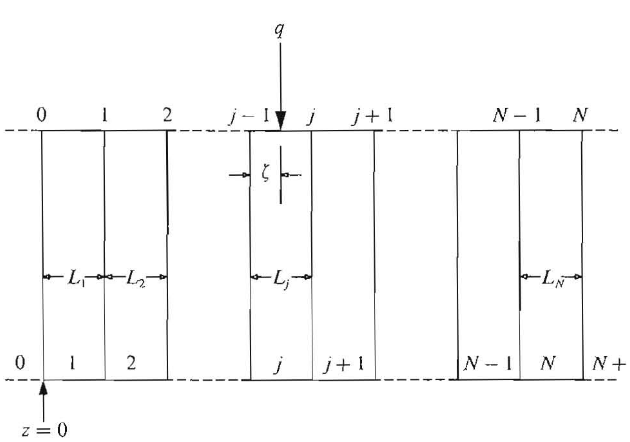

Figure 2. General multilayer system. The numbers at the top denote the boundary indices, the numbers near the bottom denote the media indices, L_j denotes the layer width, and q denotes the heat input a distance ζ from the left layer boundary.

Before proceeding with the solution, let us define some nomenclature. If we have N slabs of finite thickness with media to the right and to the left of the slab stack, there will be $N+2$ media and $N+1$ interfaces. We begin counting media from the left starting with 0 and ending with $N+1$ to the right. Each interface takes the label of the medium immediately to its left. The origin ($z = 0$) is placed at interface 0. The coordinate of interface j is z_j and the thickness of layer j is L_j. The coordinate of a heat source in layer j is $z = z_{j-1} + \zeta$, where ζ is the distance from the left boundary of medium j. We define $T_0 = T_0^{-}(0)$ and $T_{N+1} = T_{N+1}^{-}(z_N)$ for brevity.

The solution is obtained by first selecting the exterior temperature at a point adjacent to the left side of boundary 0 to be

$$\boldsymbol{T}_0 = T_0\begin{pmatrix}1\\0\end{pmatrix} , \tag{12}$$

and the exterior temperature at a point adjacent to the right side of boundary $N+1$ to be

$$\boldsymbol{T}_{N+1} = T_{N+1}\begin{pmatrix}0\\1\end{pmatrix} . \tag{13}$$

This choice insures that $T(\pm\infty) = 0$. The temperature just to the left of the heat source can be obtained if we successively apply the operations of equations (6) and (8) to equation (12). This temperature is:

$$\boldsymbol{T}_j(z_{j-1} + \zeta^-) = T_0\begin{pmatrix}A^+\\A^-\end{pmatrix} , \tag{14}$$

where A^+ and A^- are the components of a vector $\boldsymbol{A}$ given by

$$\boldsymbol{A} = \mathbf{U}_j(\zeta) \times \boldsymbol{\Gamma}_{j,j-1} \times \ldots \times \boldsymbol{\Gamma}_{3,2} \times \mathbf{U}_2(L_2) \times \boldsymbol{\Gamma}_{2,1} \times \mathbf{U}_1(L_1) \times \boldsymbol{\Gamma}_{1,0} \times \begin{pmatrix}1\\0\end{pmatrix} . \tag{15}$$

The temperature just to the right of the heat source can be obtained if we successively apply the operations of equations (6) and (8) to equation (13). This temperature is:

$$\boldsymbol{T}_j(z_{j-1} + \zeta^+) = T_{N+1}\begin{pmatrix}B^+\\B^-\end{pmatrix} , \tag{16}$$

where B^+ and B^- are the components of a vector $\boldsymbol{B}$ given by

$$\begin{aligned}\boldsymbol{B} = {}& \mathbf{U}_j(\zeta - L_j) \times \boldsymbol{\Gamma}_{j,j+1} \times \mathbf{U}_{j+1}(-L_{j+1}) \times \boldsymbol{\Gamma}_{j+1,j+2} \times \ldots \times \boldsymbol{\Gamma}_{N-2,N-1} \times \mathbf{U}_{N-1}(-L_{N-1}) \\ & \times \boldsymbol{\Gamma}_{N-1,N} \times \mathbf{U}_N(-L_N) \times \boldsymbol{\Gamma}_{N,N+1} \times \begin{pmatrix}0\\1\end{pmatrix} .\end{aligned} \tag{17}$$

The components of $\boldsymbol{A}$ and $\boldsymbol{B}$ are composed solely of specimen parameters. If we insert equations (14) and (16) into equation (11) we obtain two equations with two unknowns with the solutions:

$$T_0 = \frac{q}{2\gamma_j}\,\frac{B^+ + B^-}{A^+B^- - A^-B^+} \tag{18}$$

and

$$T_{N+1} = \frac{q}{2\gamma_j}\,\frac{A^+ + A^-}{A^+B^- - A^-B^+} . \tag{19}$$

The temperatures in all the layers can be obtained from T_0 and T_{N+1} by successive applications of the vector relationships, equations (6) and (8).

If there are heat sources at two or more coordinates, we solve for the temperature due to each source and then sum the solutions. In the case of a heat source distributed along z, the solution obtained above can be used as the Green function for obtaining the complete solution.

The above procedure is also applicable to multilayer systems in which the heat source varies in a plane parallel to the layer surfaces and/or in which the layers are finite in extent and have congruent cross-sections. In the case of finite-sized layers, heat losses from the layer edges must be negligible. In the case of infinite layers, the procedure gives an appropriate spatial transform of the temperature as a function of z and as a function of the corresponding spatial transform of the heat distribution. Fourier or Hankel transforms are typically used. In the case of finite-sized layers, the procedure gives the discrete coefficients of the appropriate spatial series expansion of the temperature as a function of z and as a function of the corresponding series expansion coefficients of the heat source. A Fourier series is typical.

4 Sample calculation

Thermal waves have been used to probe for delamination of a diamond film on a tungsten carbide substrate (Feldman 1997). The AC surface temperature of a film, heated by a modulated laser beam, was measured at the position of the heated spot as the spot was scanned across the specimen. The one-dimensional procedure described above proved to be useful for analyzing this system. As an example, we describe the procedure for calculating the top surface temperature, T_0 (equivalent to the left surface temperature in figure 2) of a similar system consisting of four media ($N = 2$): air (medium 0), film (medium 1), air gap (medium 2), and substrate (medium 3). In the earlier work (Feldman 1997) a thermal resistance was added between medium 1 and medium 2.

We assume that the modulated heat source is located in medium 1 adjacent to the boundary with medium 0; we want to know how the magnitude and phase of the temperature at the film surface vary with air gap thickness. First we calculate $\boldsymbol{A}$ by applying equation (15) which guides us to make a temperature transformation across boundary 0 to the right, using equation (8). Thus,

$$\begin{pmatrix} A^+ \\ A^- \end{pmatrix} = \frac{1}{2\gamma_1}\begin{pmatrix} \gamma_1+\gamma_0 & \gamma_1-\gamma_0 \\ \gamma_1-\gamma_0 & \gamma_1+\gamma_0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2\gamma_1}\begin{pmatrix} \gamma_1+\gamma_0 \\ \gamma_1-\gamma_0 \end{pmatrix} . \tag{20}$$

Next we calculate $\boldsymbol{B}$ by applying equation (15). We utilize the following temperature transformations: starting from medium 3, a transformation across boundary 2 to the left, using equation (9); a transformation across layer 2 to the left using equation (7); a transformation across boundary 1 to the left using equation (8); and a transformation across layer 1 to the left using equation (7). We obtain:

$$\begin{aligned}
\begin{pmatrix} B^+ \\ B^- \end{pmatrix} &= \begin{bmatrix} \exp(-u_1L_1) & 0 \\ 0 & \exp(u_1L_1) \end{bmatrix} \\
&\quad \times \frac{1}{2\gamma_1}\begin{pmatrix} \gamma_1+\gamma_2 & \gamma_1-\gamma_2 \\ \gamma_1-\gamma_2 & \gamma_1+\gamma_2 \end{pmatrix}\begin{bmatrix} \exp(-u_2L_2) & 0 \\ 0 & \exp(u_2L_2) \end{bmatrix} \\
&\quad \times \frac{1}{2\gamma_2}\begin{pmatrix} \gamma_2+\gamma_3 & \gamma_2-\gamma_3 \\ \gamma_2-\gamma_3 & \gamma_2+\gamma_3 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= \frac{1}{4\gamma_1\gamma_2}\left\{ \begin{matrix} [(\gamma_1+\gamma_2)(\gamma_2-\gamma_3)\exp(-u_2L_2)+(\gamma_1-\gamma_2)(\gamma_2+\gamma_3)\exp(u_2L_2)]\exp(-u_1L_1) \\ [(\gamma_1-\gamma_2)(\gamma_2-\gamma_3)\exp(-u_2L_2)+(\gamma_1+\gamma_2)(\gamma_2+\gamma_3)\exp(u_2L_2)]\exp(u_1L_1) \end{matrix} \right\} .
\end{aligned} \tag{21}$$

By substituting these results into equation (18) we obtain T_0. The magnitude of the thermal signal is given by $|T_0|$ and the phase is given by $\arctan(-\Im T_0/\Re T_0)$, where $\Im T_0$ is the imaginary part of T_0 and $\Re T_0$ is the real part of T_0. Because of the many terms in the expressions obtained, one usually calculates these terms numerically. In the earlier work (Feldman 1997) theoretical curves of the magnitude and phase versus air gap thickness for the solution presented here as well as for the solution that includes a thermal resistance layer were presented.

5 Conclusion

We have demonstrated a useful algorithm for solving the thermal diffusion equation in one dimension for a stratified medium that contains a modulated heating source at an arbitrary point; interface thermal resistance is easily incorporated into the calculation. The main advantage of this algorithm is its simplicity and directness. The procedure can be applied to media with thermal conductivity gradients if the gradient is normal to the specimen surfaces; in this case the media can be decomposed into sublayers of uniform composition. If the heat source is distributed through the layer thicknesses, the solution for a point source is the Green function that can be used for the full calculation. A calculation of the surface temperature of a delaminated film on a substrate demonstrated the utility of the method.

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