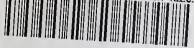


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December 1996



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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 algorithm is presented for the solution of the one dimensional thermal diffusion equation in a stratified medium containing a modulated heating source. In this context, media with thermal conductivity (or diffusivity) gradients normal to the specimen surfaces can be considered stratified media. Interface thermal resistance is easily incorporated into the calculation. In the case of heat sources varying in the x - y plane parallel to the layers, the procedure can be used to find the x - y Fourier transform of the temperature. In the case of a multilayer stack of rectangular cross section, the procedure can be used to find the coefficients of the x - y Fourier series expansion of the temperature. A sample calculation for a delaminated diamond film on a WC substrate is presented.

Key words: diamond film, heat diffusion, multilayer, stratified medium, thermal diffusion, thermal waves

ALGORITHM FOR SOLUTIONS OF THE THERMAL DIFFUSION EQUATION IN A STRATIFIED MEDIUM WITH A MODULATED HEATING SOURCE

1. Introduction

The solutions of the thermal diffusion equation in a stratified (multilayer) medium are important for many modern applications such as thermal diffusivity measurements¹, thermal wave nondestructive probes², heat conduction in optical disk recording³, and heat dissipation in electronic multilayer structures⁴. Several analyses have been made of ac⁵ or dc steady state heat flow in general multilayer systems^{4,6}, however, they have included either no heat source⁶ or a heat source at an outer surface^{4,5}.

This paper presents a simple 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 used involves a simple matrix formalism that is analogous to that given in Carslaw and Jaeger⁶. Thermal resistance at each interface is easily incorporated into the solution. The solution for heat sources distributed normal to the specimen surfaces is obtained by using the discrete plane source as the Green function.

Recently, several papers have treated the propagation of thermal waves in linearly inhomogeneous materials^{7,8} with the thermal conductivity (diffusivity) gradient normal to the specimen surfaces. From a computational point of view, the procedure presented in this note can easily treat any profile as a series of uniform layers. We present a sample calculation for a delaminated diamond film on a WC substrate.

The procedure is also applicable to solving a wider range of problems: 1) Layered systems containing heating sources distributed in the x - y plane parallel to the layers. The procedure yields the x - y spatial Fourier transform of the temperature distribution. 2) Layered systems having a rectangular cross section. The procedure yields the coefficients of the x - y spatial Fourier series expansion of the temperature.

2. Matrix formulation

The one dimensional homogeneous differential equation that describes heat diffusion for a modulated heating source of angular frequency ω is,

$$\frac{d^2T}{dz^2} + i\frac{\omega}{D}T = 0, \quad (1)$$

where D is the thermal diffusivity and T is the complex temperature at ω . The time dependence is $e^{-i\omega t}$. We assume that D for any medium in the problem is homogeneous, isotropic, and independent of T . The heat source has not been included in the equation; instead, heating is treated as a boundary condition. The solutions can be written as the sum of exponentials that are growing (+) and decaying (-) in the positive z direction,

$$T(z) = T^+ e^{uz} + T^- e^{-uz}, \quad (2)$$

where, $u^2 = -i \frac{\omega}{D}$, and T^+ and T^- constants to be determined. The solutions to eq. (2) can also be expressed in the form of waves, called thermal waves, if we make the substitution $u = iw$.

The temperature can be treated as a two dimensional vector \mathbf{T} given by

$\mathbf{T} = \begin{pmatrix} T^+(z) \\ T^-(z) \end{pmatrix} = \begin{pmatrix} T^+ e^{uz} \\ T^- e^{-uz} \end{pmatrix}$. Consider a boundary plane at $z = \xi$ between media a and b , as seen in figure 1, with no heating in the vicinity of the boundary. The temperature and heat flow are continuous across the boundary, thus

$$T_a(\xi^-) = T_b(\xi^+), \quad (3)$$

$$\kappa_a \left. \frac{dT_a}{dz} \right|_{z=\xi^-} = \kappa_b \left. \frac{dT_b}{dz} \right|_{z=\xi^+}, \quad (4)$$

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. Inserting the solution eq. (2) into eqs. (3) and (4), we obtain

$$T_a^+(\xi^-) + T_a^-(\xi^-) = T_b^+(\xi^+) + T_b^-(\xi^+), \quad (5)$$

$$\gamma_a T_a^+(\xi^-) - \gamma_a T_a^-(\xi^-) = \gamma_b T_b^+(\xi^+) - \gamma_b T_b^-(\xi^+), \quad (6)$$

where $\gamma_j = u_j \kappa_j$.

Equations (5) and (6) can be represented as a matrix equation

$$\mathbf{T}_b = \Gamma_{ba} \mathbf{T}_a, \quad (7)$$

where

$$\Gamma_{ba} = \frac{1}{2\gamma_b} \begin{pmatrix} \gamma_b + \gamma_a & \gamma_b - \gamma_a \\ \gamma_b - \gamma_a & \gamma_b + \gamma_a \end{pmatrix}. \quad (8)$$

Equation (7) relates the temperature on two sides of an interface.

If the interface between two media contains a thermal resistance, R [ref. 6], then eq.

(8) becomes

$$\Gamma_{ba} = \frac{1}{2\gamma_b} \begin{pmatrix} \gamma_b + \gamma_a + \gamma_b \gamma_a R & \gamma_b - \gamma_a - \gamma_b \gamma_a R \\ \gamma_b - \gamma_a + \gamma_b \gamma_a R & \gamma_b + \gamma_a - \gamma_b \gamma_a R \end{pmatrix}. \quad (8a)$$

The relationship between the temperatures at two points in a given medium a separated by a distance $L = z_j - z_i$ with no intervening heat source is

$$\mathbf{T}_a(z_j) = \mathbf{U}_a(L) \mathbf{T}_a(z_i), \quad (9)$$

where,

$$\mathbf{U}_a(L) = \begin{pmatrix} e^{uL} & 0 \\ 0 & e^{-uL} \end{pmatrix}. \quad (10)$$

Thus, eqs. (7) and (9) allow us to express the temperature at any coordinate as a function of the temperature at any other coordinate, provided there is no intervening heat source.

If heat is applied uniformly to the boundary at a rate $q \text{ W cm}^{-2}$, then eq. (4) becomes

$$\kappa_a \left. \frac{dT_a}{dz} \right|_{z=\xi^-} = \kappa_b \left. \frac{dT_b}{dz} \right|_{z=\xi^+} + q, \quad (11)$$

and the matrix equation becomes

$$\mathbf{T}_b = \Gamma_{ba} \mathbf{T}_a - \frac{q}{2\gamma_b} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (12)$$

If the heating occurs within a single medium, eq. (12) simplifies considerably ($\Gamma = \mathbf{1}$, the identity matrix); thus, when performing calculations, it is most convenient to consider heating to occur within a single medium. 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. One dimensional multilayer heat flow

Consider a multilayer system as seen in figure 2. We want to solve for the temperature at every point (or plane) for heat input at any particular point (or plane).

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, 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 nomenclature for the temperature vector at any plane z located in medium j is $T_j(\zeta)$, where ζ is the distance from the left boundary of medium j , that is, $z=z_{j-1}+\zeta$. For brevity, we define $T_0^+=T_0^+(0)$ and $T_{N+1}^- = T_{N+1}^-(z_{N+1})$.

Now, let us consider the temperature vector relationship in the vicinity of the heat source. Because a single medium surrounds the source, eq. (12) simplifies to

$$T_j(\zeta^+) - T_j(\zeta^-) = -\frac{q}{2\gamma_j} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (13)$$

In medium 0, the temperature must remain finite in the limit, $z \rightarrow -\infty$, thus, $T_0^-(z)=0$, whereas in medium $N+1$, the temperature must remain finite in the limit, $z \rightarrow \infty$; thus, $T_{N+1}^+ = 0$. Hence one can easily show that $T_j^+(\zeta^-)$ and $T_j^-(\zeta^-)$ are both proportional to T_0^+ and $T_j^+(\zeta^+)$ and $T_j^-(\zeta^+)$ are both proportional to T_{N+1}^- . If $T_j^-(\zeta^-) = A^+ T_0^+$, $T_j^-(\zeta^-) = A^- T_0^+$; $T_j^+(\zeta^+) = B^+ T_{N+1}^-$, and $T_j^+(\zeta^+) = B^- T_{N+1}^-$ then eq. (13) becomes

$$T_{N+1}^- \mathbf{B} - T_0^+ \mathbf{A} = -\frac{q}{2\gamma_j} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad (14)$$

where, $\mathbf{A} = \begin{pmatrix} A^+ \\ A^- \end{pmatrix}$ and $\mathbf{B} = \begin{pmatrix} B^+ \\ B^- \end{pmatrix}$. Equation (14) represents two simultaneous equations that can be solved for T_0^+ and T_{N+1}^- . The solutions are

$$T_0^+ = \frac{q}{2\gamma_j} \frac{B^+ + B^-}{A^+ B^- - A^- B^+} \quad (15)$$

$$T_{N+1}^- = \frac{q}{2\gamma_j} \frac{A^+ + A^-}{A^+ B^- - A^- B^+} \quad (16)$$

The temperatures in all of the layers can be obtained from T_0^+ and T_{N+1}^- by successive applications of the vector relationships eqs. (7) and (9).

4. General Procedure

To solve for the temperature distribution throughout the multilayer stack for a heat source at position $z=z_{j-1}+\zeta$, we must first solve for the components of the vectors \mathbf{A} and \mathbf{B} . These are given by

$$\mathbf{A} = \mathbf{U}_f(\zeta) \times \Gamma_{j,j-1} \times \dots \times \Gamma_{3,2} \times \mathbf{U}_2(L_2) \times \Gamma_{2,1} \times \mathbf{U}_f(L_1) \times \Gamma_{1,0} \times \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad (17)$$

$$\begin{aligned} \mathbf{B} = & \mathbf{U}_f(\zeta - L_j) \times \Gamma_{j,j+1} \times \mathbf{U}_{j+1}(-L_{j+1}) \times \Gamma_{j+1,j+2} \times \dots \\ & \dots \times \Gamma_{N-2,N-1} \times \mathbf{U}_{N-1}(-L_{N-1}) \times \Gamma_{N-1,N} \times \mathbf{U}_N(-L_N) \times \Gamma_{N,N+1} \times \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned} \quad (18)$$

By inserting the components of \mathbf{A} and \mathbf{B} into eqs. (15) and (16), we obtain the temperatures at the outer surfaces of the multilayer stack. Successive applications of eqs. (7) and (9) allow us to obtain the temperature at any location within the stack. If heating occurs at an interface between two media, such as to position $z = z_{j-1}$, we just take the limit as $\zeta \rightarrow 0$.

If there are heat sources at two or more coordinates, we solve for the temperature for each source separately 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 solution.

5. Spatially Varying Heat Source in a Multilayer System

In the previous discussion, we assumed that heat was applied to a plane uniformly. Let us now assume a planar heat source that is varying in the xy plane exists at $z = \zeta$, that is, $q = q(x, y)$. The heat diffusion equation in cartesian coordinates for three dimensional heat flow is given by

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + i \frac{\omega}{D} T = 0. \quad (19)$$

The general solution for each layer in a multilayer system is of the form

$$T_j(x, y, z) = \int \int_{-\infty-\infty}^{\infty} \left\{ \tilde{T}_j^+(k_x, k_y, z) + \tilde{T}_j^-(k_x, k_y, z) \right\} e^{ik_x x} e^{ik_y y} dk_x dk_y, \quad (20)$$

where,

$$\tilde{T}_j^+(k_x, k_y, z) = c_j^+(k_x, k_y) e^{u_j z}, \quad (21)$$

$$\tilde{T}_j^-(k_x, k_y, z) = c_j^-(k_x, k_y) e^{-u_j z}, \quad (22)$$

and

$$u_j = \left(k_x^2 + k_y^2 - i \frac{\omega}{D_j} \right)^{1/2}. \quad (23)$$

If we see that the temperature is the inverse two dimensional Fourier transform of two terms. The two dimensional Fourier transform of $q(x,y)$ can be written as

$$\bar{q}(k_x, k_y) = \frac{1}{(2\pi)^2} \int \int_{-\infty-\infty}^{\infty \infty} q(x,y) e^{-ik_x x} e^{-ik_y y} dx dy \quad (24)$$

If we match the boundary conditions at an interface between two layers using eqs. (20) and (24), we obtain a matrix equation of the same form as eq. (12) with Fourier transforms of the temperature and the heat source replacing the temperature and heat source of the one dimensional case. In addition, eqs. (21) and (22) have the same form as the terms in eq. (2). Thus, the formalism developed for the one dimensional case can be seen to apply directly to the Fourier transforms of the higher dimensional case. In the case of an axially symmetric heat source in the xy plane, the formalism holds as well except that we must use Hankel transforms instead of Fourier transforms.

6. Multilayer System with Rectangular Cross-Section

The procedure described above also applies to a buried planar heat source in a multilayer system having a rectangular cross-section of dimensions L_x and L_y . In this case the above procedure can be used to solve for the coefficients of the Fourier series analogous to that given by eq. (15) in reference 4. In this case we assume heat loss from the edges of the films is negligible compared to loss through the end faces of the stack and, therefore, can be ignored.

7. Sample calculation

Thermal waves can be used to probe for delamination of a thin film on a substrate and the one dimensional formalism is useful for analyzing this system. The system consists of an air ambient (medium 0), a film (medium 1), an air gap (medium 2) of varying thickness, and a substrate (medium 3); $N=2$. We assume that the modulated heat source is in medium 1 at the boundary with medium 0; we want to know how the magnitude and phase of the temperature at the film surface vary as a function of the air gap thickness. From eqs. 17 and 18 we obtain

$$A^+ = \frac{\gamma_1 + \gamma_0}{2\gamma_1}, \quad (25)$$

$$A^+ = \frac{\gamma_1 - \gamma_0}{2\gamma_1}, \quad (26)$$

$$B^+ = \frac{(\gamma_1 + \gamma_2)(\gamma_2 - \gamma_3)e^{-u_2 L_2} + (\gamma_1 - \gamma_2)(\gamma_2 + \gamma_3)e^{u_2 L_2}}{4\gamma_1 \gamma_2} e^{-u_1 L_1}, \quad (27)$$

and

$$B^- = \frac{(\gamma_1 - \gamma_2)(\gamma_2 - \gamma_3)e^{-u_2 L_2} + (\gamma_1 + \gamma_2)(\gamma_2 + \gamma_3)e^{u_2 L_2}}{4\gamma_1 \gamma_2} e^{u_1 L_1}. \quad (28)$$

Inserting these into eq. 15, we obtain the surface temperature T_0^+ .

The magnitude of the thermal signal is given by $|T_0^+|$, and the phase is given by $\arctan(-\Im T_0^+ / \Re T_0^+)$. Figure 3 shows a plot of the magnitude and phase of the thermal signal as a function of air gap thickness at a modulation frequency of 200 Hz for a delaminated film of diamond 20 μm thick on a tungsten carbide substrate. Table 1 lists the material parameters used in the computation.

8. Conclusion

We have demonstrated a straightforward algorithm for solving the thermal diffusion equation in one dimension for a stratified medium with a modulated heating source. It 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. Interface thermal resistance is easily incorporated into the calculation. If the heat source has a spatial variation in the x - y plane parallel to the layers, the procedure can be used to obtain the x - y spatial Fourier transforms of the temperature distribution. In the case of a multilayer stack of rectangular cross section, the procedure can be used to solve for the coefficients of the x - y Fourier series expansion of the temperature. A sample calculation for a delaminated diamond film on a WC substrate was presented.

7. References

1. M. Reichling and H. Grönbeck, *J. Appl. Phys.* **75**, 1914 (1994).
2. J.W.M. Spicer, W.D. Kerns, L.C. Aamodt, R. Osiander, and J.C. Murphy, "Time-Resolved Infrared Radiometry (TRIR) using a Focal Plane Array for Characterization of Hidden Corrosion", in *Thermosense XV*, L.R. Allen, Editor, Proc. SPIE **1933**, 149 (1993).
3. O.W. Shih, *J. Appl. Phys.* **78**, 6397 (1995).
4. J. Albers, *IEEE Trans. on Components, Packaging, and Manufacturing Technology—Part A*, **18**, 31 (1995).
5. A.G. Kokkas, *IEEE Trans. Electron. Devices*, **ED-21**, 674 (1974).
6. H.S. Carslaw and J.C. Jaeger, *Conduction of Heat in Solids* (Oxford University Press, London, 1959) p. 111.
7. J. Fivez and J. Thoen, *J. Appl. Phys.* **75**, 7696 (1994)
8. J. Fivez and J. Thoen, *J. Appl. Phys.* **79**, 2225 (1996)

Table 1. Numerical Parameters Used in the Example

medium	κ (W cm ⁻¹ K ⁻¹)	ρ (g cm ⁻³)	C (J g ⁻¹ K ⁻¹)
0, 2	0.00026	0.00129	1.01
1	9.6	3.5	0.51
3	0.95	15.	0.28

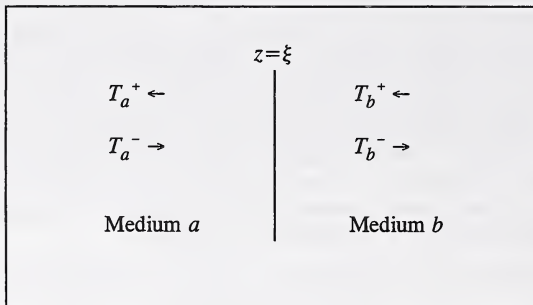


Figure 1. Heating at a boundary between two media.

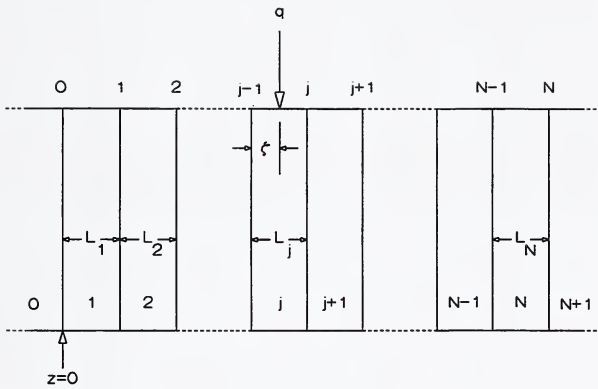


Figure 2. General multilayer system. The numbers at the top denote the boundary indices, the numbers near the bottom denote the media indices, L_j denotes the layer width, and q denotes the heat input a distance ζ from the left layer boundary.

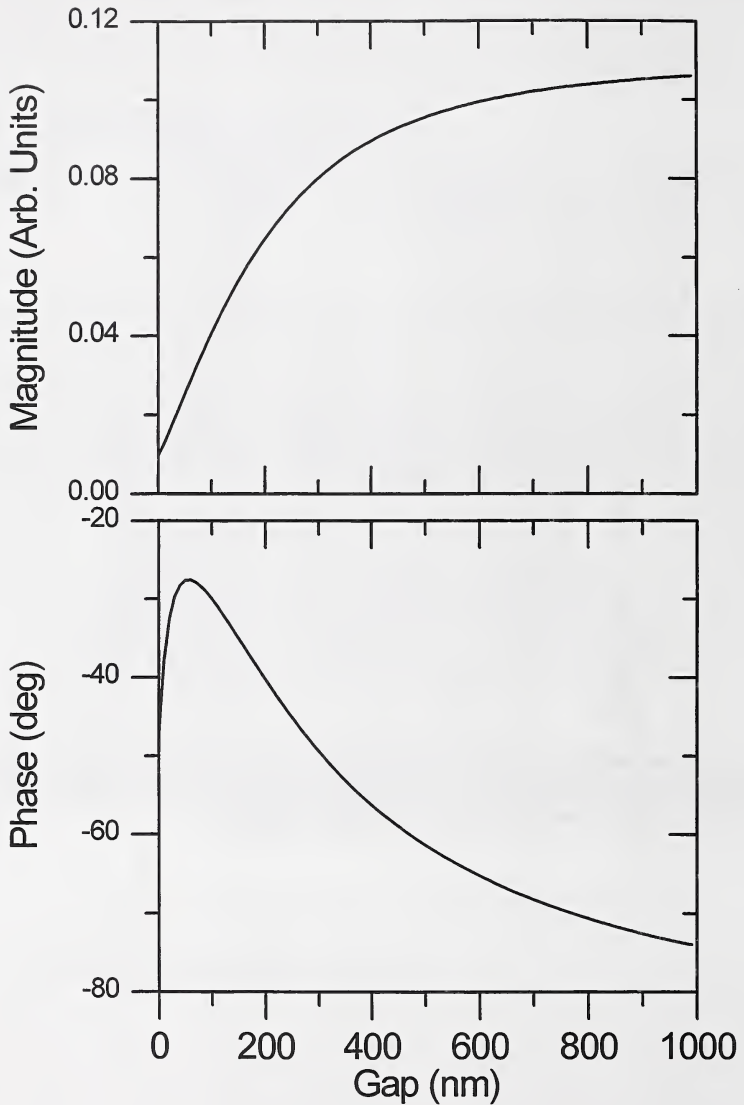


Figure 3. Magnitude and phase of the thermal signal as a function of air gap thickness at a modulation frequency of 200 Hz for a film of diamond $20\mu\text{m}$ thick on a tungsten carbide substrate. Table 1 lists the material parameters used in the computation.

