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# A General Solution to the One- and Two-Dimensional Melting Using a Finite Difference Approach

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## ABSTRACT

A general solution has been developed for the melting of solid materials, including a phase transition in the one- and two-dimensional models requiring a minimal amount of computer time and space and using a nonstandard finite difference approach. Accuracies of 1% in temperature profiles with time can easily be achieved. Both of these programs will handle a wide range of heating power levels and any desired thickness of liquid layer retained.

Techniques developed in the one-dimensional case have served as helpful guidelines for the more complex two-dimensional geometry. Similarly, comparisons of the one- and two-dimensional burn-through times and temperature profiles have aided in separating out the effects of radial heat conduction and geometry.

## PROBLEM STATUS

This is a final report on this phase of the problem; work on other phases of the problem is continuing.

## AUTHORIZATION

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## A GENERAL SOLUTION TO THE ONE- AND TWO-DIMENSIONAL MELTING USING A FINITE DIFFERENCE APPROACH

### INTRODUCTION

Two programs have been developed to solve the melting of solid materials including a phase transition in both the one- and two-dimensional models. Both of these programs will handle a wide range of heating power levels and any desired thickness of liquid layer retained.

The technique employed in these programs is an unconventional finite difference technique in which the fusion front position is treated continuously, and, presently only in the one-dimensional program, a sixth-order, space-time expansion is employed in both the heat diffusion equation and the fusion front position equation.

Techniques developed in the one-dimensional case have served as helpful guidelines for the more complex two-dimensional geometry. Similarly, comparisons of the one- and two-dimensional burn-through times and temperature profiles have aided in separating out the effects of radial heat conduction and geometry.

The finite difference formalation is convenient for treating a variety of power levels and types of materials with widely varying thermal constants since one need only change input parameters rather than alter the program.

Accuracies of 1% have been easily obtained in the one-dimensional burn-through times as compared to an exact expression for total burn-through time in the limit of ablation (1) and temperature profiles as compared with exact premelting solutions (2). Good agreement has also been obtained between the one- and two-dimensional programs in the appropriate limiting case of a flat slab.

### FORMULATION OF EQUATIONS

Consider the one-dimensional heat diffusion equation

$$\frac{\partial T}{\partial t} = \alpha^2 \frac{\partial^2 T}{\partial X^2} \quad (1)$$

Let the temperature  $T$  have space and time coordinates  $i$  and  $j$ , respectively. Then the conventional finite difference approximation for this equation is

$$\frac{1}{\Delta t} [T(i, j+1) - T(i, j)] = \frac{\alpha^2}{\Delta X^2} [T(i+1, j) - 2T(i, j) + T(i-1, j)]. \quad (2)$$

In place of Eq. (2), a seven-point expansion is used to evaluate the second-order derivative giving an equation of the form

$$\begin{aligned}
\frac{1}{\Delta t} [T(i, j+1) - T(i, j)] &= a'_1 [T(i, j-1) - T(i, j)] \\
&+ a'_2 [T(i-1, j-1) - 2T(i, j) + T(i+1, j-1)] \\
&+ a'_3 [T(i-1, j) - 2T(i, j) + T(i+1, j)], \tag{3}
\end{aligned}$$

where  $a'_1$ ,  $a'_2$ , and  $a'_3$  are known functions of the thermal parameters of the material (Appendix C). The boundary condition at the front surface is

$$K\nabla T = \alpha_m H_0 \tag{4}$$

and the standard finite difference approximation to Eq. (4) is

$$T(i, j) = T(i+1, j) + \frac{\alpha_m H_0 \Delta X}{K}. \tag{5}$$

It should be emphasized that  $\alpha_m H_0$  is the power absorbed by the material and not the incident power. Knowledge of the absorption coefficient  $\alpha_m$  for the wavelength and material considered is important (3, 4).

Once the front surface is brought up to melting temperature, a second boundary condition must be applied to the liquid/solid interface:

$$F \frac{\partial m}{\partial t} = K\nabla T \Big|_{x_m^-} - K\nabla T \Big|_{x_m^+}, \tag{6}$$

where  $F$  is the latent heat of fusion of the material and  $x_m$  is the position of the fusion interface. A simple two-point approximation to the gradient gives

$$x_m(j+1) = x_m(j) + \frac{K\Delta t}{\rho F \Delta X} [T(i-1, j) - 2T(i, j) + T(i+1, j)]. \tag{7}$$

In place of Eq. (7) a seven-point expansion has been substituted:

$$\begin{aligned}
x_m(j+1) &= x_m(j) + b'_1 [T(i-1, j-1) - 2T(i, j) \\
&+ T(i+1, j-1)] + b'_2 [T(i, j+1) - T(i, j-1)] \\
&+ b'_3 [T(i-1, j) - 2T(i, j) + T(i+1, j)]. \tag{8}
\end{aligned}$$

Here  $b'_1$ ,  $b'_2$ , and  $b'_3$  are known functions of the thermal constants of the material (Appendix C).

The condition at the back wall used here is that there is no heat flow, which corresponds to an insulated slab; i.e.,

$$K\nabla T = 0. \tag{9}$$

Thus, the last two lattice points are given by

$$T(i, j) = T(i-1, j). \tag{10}$$

## TWO-DIMENSIONAL PROGRAM

The two-dimensional program is designed to treat a cone of arbitrary vertex angle and of any material. The thickness and number of subdivisions are completely general. In the two-dimensional program the temperature gradients are no longer directed along the lattice rows as in the simplified one-dimensional program. The two-dimensional heat conduction equation is now used, and the program sets up a lattice array for the input cone angle such that lattice points fall on the front and back surface. This feature greatly simplifies the computational complexity of the program.

The thermal gradients are set equal to zero along the top and bottom lattice rows and at the back surface. Cosine attenuation of the incident power is used at all front surface points except the vertex point, which receives direct irradiation. The thermal gradient direction for the melt interface is directed along the lattice row behind the vertex point and varies linearly until it becomes normal to the front surface at the top and bottom rows. An outline of the two-dimensional program appears in Appendix B.

## ONE-DIMENSIONAL RESULTS

The one-dimensional results are given in Figs. 1 through 7 in the form of temperature profiles.

## TWO-DIMENSIONAL RESULTS

The top half of Fig. 8 shows a two-dimensional aluminum cone with a 60-degree half angle. Burn-through occurs first at the region away from the tip of the cone, due to the fact that the greater distance the melt must travel at the tip outweighs and cosine attenuation of the beam away from the tip. The burn-through at the tip does occur at 8.6 seconds. A comment should be made here that due to the formatting of the output all temperatures are rounded off to the nearest whole degree. This does not reflect the accuracy of the program.

The lower half of Fig. 8 shows the 60-degree half-angle cone at 6.79 seconds just after burn-through has occurred at the top and bottom. The cone is nearly isothermal at this time.

Figure 9 shows a 60-degree half-angle aluminum cone with only the center five rows irradiated to study the effects of radial heat conduction. As can be seen, the heating is slowed down more than an order of magnitude by the nonirradiated portion of the cone.

An 85-degree half-angle aluminum cone is shown in Fig. 10 for comparison to the one-dimensional program. Burn-through occurs in 5.7 seconds for the two-dimensional program as compared with 5.8 seconds with the one-dimensional program.

## ACKNOWLEDGMENT

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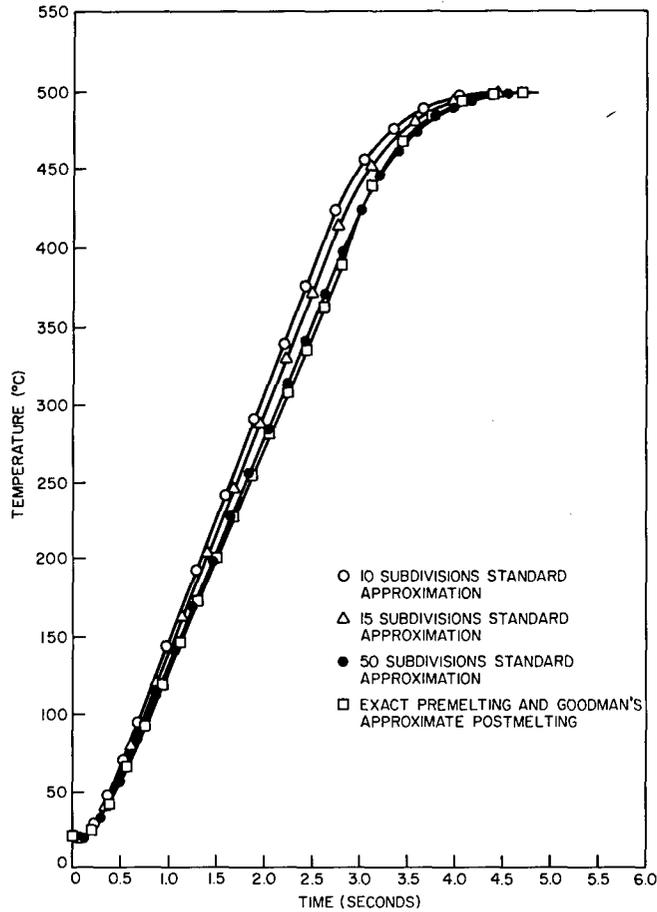


Fig. 1 - Temperature versus time at back surface of a 0.953-cm-thick slab of aluminum 2024 irradiated with 20,000 watts/cm<sup>2</sup>. The curves show improved accuracy with increased subdivisions. All of these runs were made with the standard finite difference equation, using an absorption coefficient of 0.02.

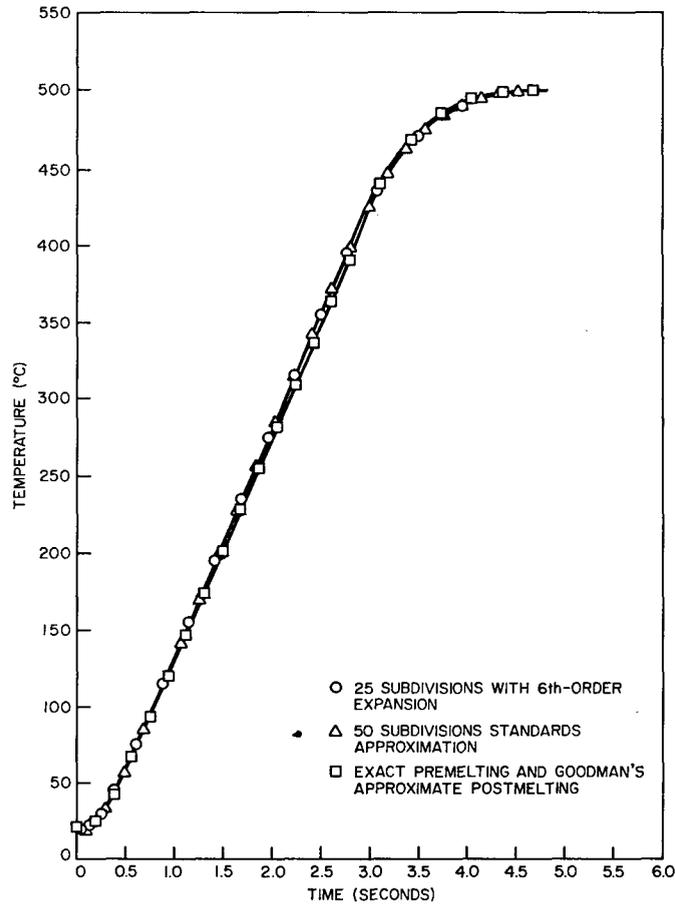


Fig. 2 - Improved accuracy of Fig. 1 as a result of introducing the sixth-order, space-time expansion for temperature. Equal accuracy for aluminum may be obtained with 25 subdivisions using the sixth-order expansion as with 50 subdivisions without the expansion.

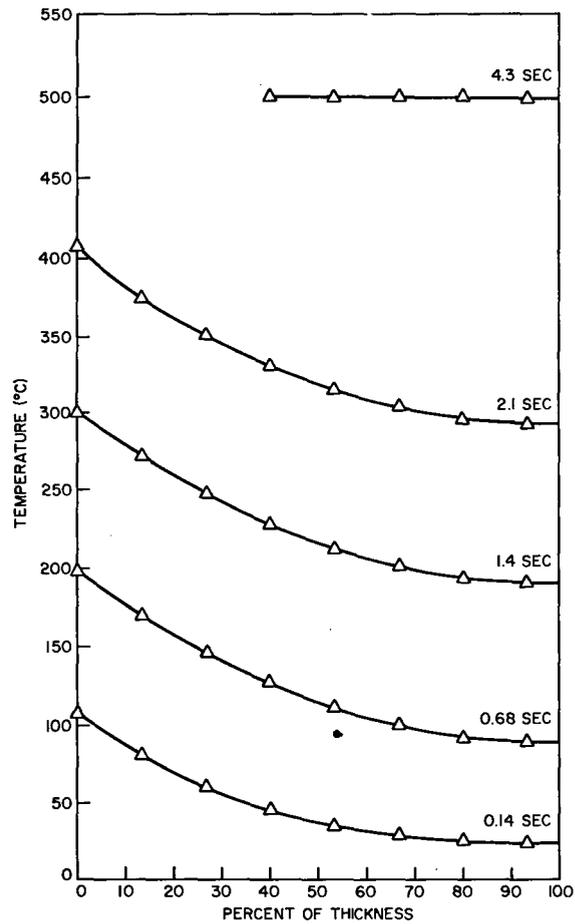


Fig. 3 - Temperature profiles at various times after the onset of irradiation of a 0.953-cm-thick slab of aluminum 2024. The irradiating power was 20,000 watts/cm<sup>2</sup>, and the absorption coefficient used was 0.02. The slab becomes nearly isothermal after ablation begins.

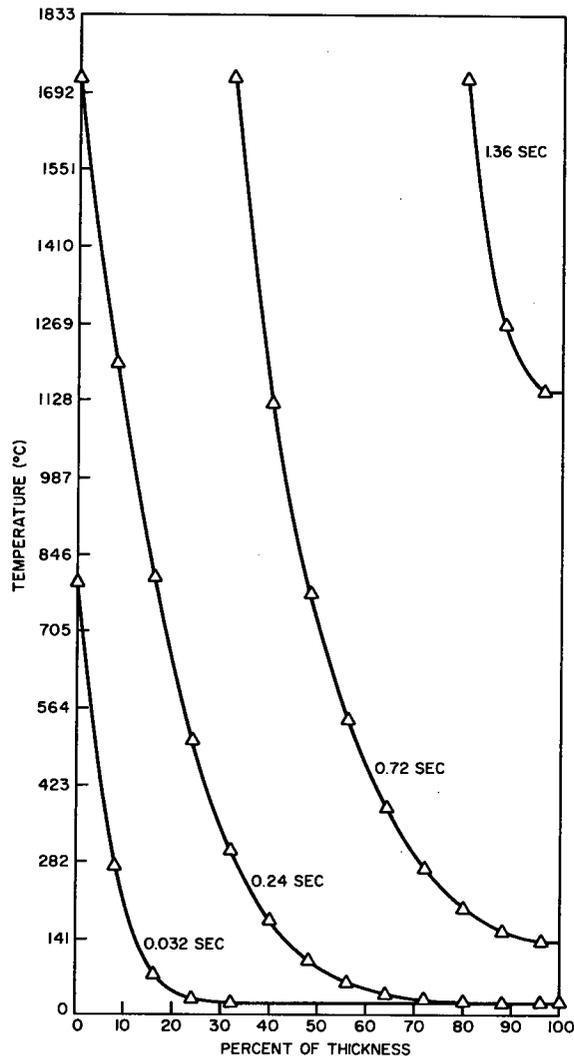


Fig. 4 - Temperature profiles in a 0.5-cm slab of stainless steel at various times after the onset of irradiation. The steep thermal gradients which occur with stainless steel, as compared to the higher thermal conductivity metal, aluminum, require more subdivisions for comparable accuracy with aluminum runs. Accuracies of 4% for stainless steel have been obtained with 50 subdivisions. Even after melting has started at the front surface, the back surface is essentially at ambient. The irradiating power was 20,000 watts/cm<sup>2</sup>, and the absorption coefficient used was 0.2.

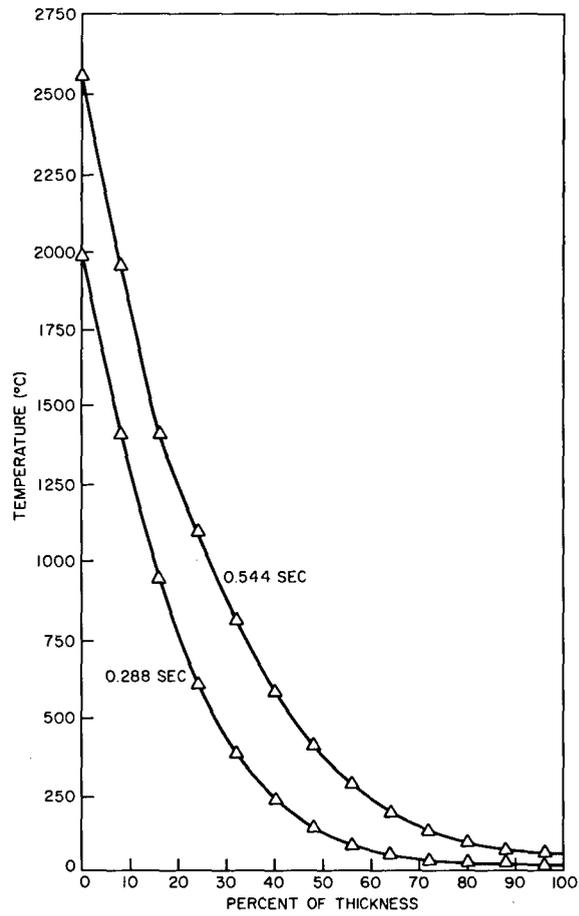


Fig. 5 - Temperature profiles at two times from onset of irradiation for a 0.5-cm slab of 304 stainless steel. The irradiating power was 20,000 watts/cm<sup>2</sup>, and the absorption coefficient used was 0.2. A 16% liquid layer retained model was used.

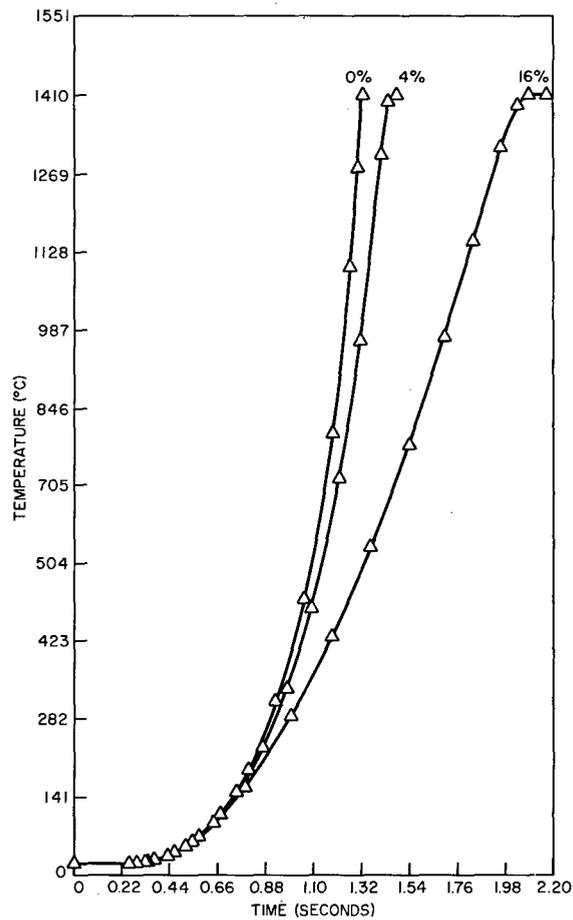


Fig. 6 - Temperature rise at the back surface of a 0.5-cm slab of 304 stainless steel for three thicknesses of liquid layer retained (0%, 4%, and 16%). The different character of these curves could be used in conjunction with experimental measurement to determine a realistic liquid layer retained for a given material and power level. The irradiating power was 20,000 watts/cm<sup>2</sup>, and the absorption coefficient used was 0.2.





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## Appendix A

## ONE-DIMENSIONAL PROGRAM

1. Thermal properties of the material, thickness of the slab, initial temperature distribution, irradiating power level, number of subdivisions to be made, liquid layer retained, and the print-out frequency are all read in.
2. A time step suitable for convergence of all expansions is calculated.
3. Evaluation of all expansion coefficient algebra is made outside the repetitive loop to increase computer efficiency.
4. Assignment of initial temperature distribution is made.
5. A liquid layer matrix is calculated which serves to interpret appropriate equations to be applied.
6. Application of heat conduction equation is made to all internal points.
7. Boundary conditions are applied to the front and back surfaces.
8. A test for the print-out frequency is made.
9. A test is made for resetting the subscripted variables if maximum size is exceeded. This step allows minimum storage requirements for the program.
10. A test for melting at the front surface is made, and if no melting has occurred, the program is recycled through step 6.
11. The fusion front is initialized at the front surface.
12. The heat conduction equation is applied to all interior points.
13. The exact position of the fusion front is evaluated.
14. The temperature at the nearest lattice point is fixed to the melting temperature.
15. The boundary conditions at the front and back surfaces are applied.
16. A test for the print-out frequency is made.
17. A test is made for the maximum array size for resetting the subscripted variables.
18. A test for burn-through is made, and if no burn-through occurs, the program is cycled back through step 12.

## Appendix B

### TWO-DIMENSIONAL PROGRAM

1. The thermal parameters of the material, thickness of material, angle of cone, initial temperature distribution, irradiating power level, number of subdivisions to be made across the thickness, the thickness of liquid layer retained, and the print-out frequency are read in.
2. The lattice array such that the front and back surfaces coincide with lattice points is set up.
3. A liquid matrix similar to that used in the one-dimensional program is set up.
4. The melt line gradient direction is set up for each row independently.
5. The irradiating power distribution cross section is set up.
6. The initial nose cone temperatures are assigned to lattice points.
7. If no melt has started, test each row independently to check for initial melting temperature at the front surface.
8. The two-dimensional heat diffusion equation for all interior points is applied.
9. The boundary conditions of no thermal gradient at the top and bottom rows are applied.
10. The position of the melt interface is calculated.
11. The boundary condition is applied to the front surface.
12. A test is made of the print-out frequency.
13. A test is made to check if burn-through has occurred.
14. A test for the maximum subscripting is made to the reset subscripts. Then a re-cycle is made through step 7.

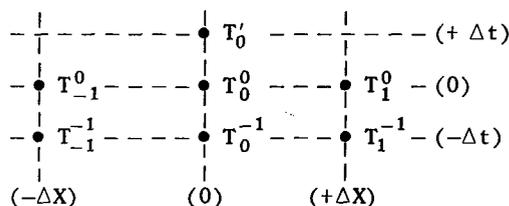
## Appendix C

## TEMPERATURE EXPANSIONS

The expansion in space and time chosen for the temperature is

$$\begin{aligned}
 T(X, t) = & a_0 + a_1 X + a_2 X^2 + a_3 X^3 + a_4 X^4 + a_5 X^5 \\
 & + a_6 X^6 + b_0 t + b_1 X t + b_2 X^2 t + b_3 X^3 t \\
 & + b_4 X^4 t + c_0 t^2 + c_1 t^3 + d_1 X t^2 + d_2 X^2 t^2.
 \end{aligned}$$

Substitution of Eq. (C1) into the heat diffusion equation gives a relationship between the coefficients. There remain the seven  $a$  coefficients as unknowns. These are solved by choosing a suitable lattice of seven points:



The above lattice was chosen because it allows the expansion to be used for all interior points of the lattice. If an expansion along the lattice row was chosen, simpler approximations would have to apply at the front and back of the lattice. On substituting Eq. (C1) into each of the above seven lattice points, seven equations are obtained which may be solved for the  $a$  coefficients.

The results of the algebra are

$$\begin{aligned}
 D1 &= -4a^2 \Delta t \\
 D2 &= -240a^6 \Delta t^3 \\
 D3 &= 2\Delta X^2 - 4a^2 \Delta t \\
 D4 &= 2\Delta X^4 - 24\Delta X^2 a^2 \Delta t + 24a^4 \Delta t^2 \\
 D5 &= 2\Delta X^6 - 60\Delta X^4 a^2 \Delta t - 240a^6 \Delta t^3 + 360\Delta X^2 a^4 \Delta t^2 \\
 D6 &= 2\Delta X^2 \\
 D7 &= 2\Delta X^4 \\
 D8 &= 2\Delta X^6
 \end{aligned}$$

$$G1 \equiv \frac{(D8 D1 - D6 D2) 24\alpha^4 \Delta t^2}{D4 (D8 D1 - D6 D2) - D7 (D5 D1 - D3 D2)}$$

$$G2 \equiv \frac{D3 (D8 D1 - D6 D2) 24\alpha^4 \Delta t^2}{D1 D4 (D8 D1 - D6 D2) - D1 D7 (D5 D1 - D3 D2)}$$

$$G3 \equiv \frac{(D5 D1 - D3 D2) 24\alpha^4 \Delta t^2}{D4 (D8 D1 - D6 D2) - D7 (D5 D1 - D3 D2)}$$

$$G4 \equiv \frac{(D5 D1 - D3 D2) D6 24\alpha^4 \Delta t^2}{D1 D4 (D8 D1 - D6 D2) - D1 D7 (D5 D1 - D3 D2)}$$

Then we have for the temperature

$$\begin{aligned} T_0^1 &= T_0^0 + \left( \frac{G4 - G2 - 1}{G4 - G2 + 1} \right) (T_0^{-1} - T_0^0) \\ &+ \frac{G1 (T_{-1}^{-1} - 2T_0^0 + T_1^{-1})}{(1 - G2 + G4)} \\ &- \frac{G3 (T_{-1}^0 - 2T_0^0 + T_1^0)}{(1 - G2 + G4)} \end{aligned}$$

## Appendix D

## NOTATIONS

The notations for the thermal constants are

$\alpha^2$	thermal diffusivity (cm <sup>2</sup> /sec)
K	thermal conductivity (cal/cm-sec-deg.C)
F	latent heat of fusion (cal/g)
$\Delta X$	spatial lattice subdivision
$\Delta t$	time subdivision
$\alpha_m$	absorption coefficient
$H_0$	incident flux (cal/cm <sup>2</sup> -sec)
$\rho$	mass density
T(X, t)	temperature at x and t

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Laser heating Melt-through times Laser damage						