Appendix A

Using the HEAT Program.

A.1 Introduction

HEAT is a DOS program package written for steady state and transient thermal modeling of three dimensional objects. A finite difference algorithm is utilized for solving the steady state temperature profiles using a Gauss-Seidel iteration technique. For transient analyses, a modified algorithm developed by Jason Lewis is used which does not involve time-stepping. The program was designed specifically for microelectronics applications which involve uniform heat dissipation within thin films on a relatively thick material. The HEAT program includes tools for viewing and filing to disk:

1) One dimensional temperature profiles parallel to the X, Y, or Z axis, at any point in the corresponding orthogonal plane.

2) Isotherm profiles in the X-Y, X-Z, or Z-Y planes at any point in the orthogonal axis.

A.2 Grid Layout

The HEAT program relies on a grid matrix of nodes to represent the region of mass being modeled. The overall region is bounded by a rectangular parallelepiped by values of X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, and Z_{max}. Each of these six boundaries is defined as either a thermal insulator or as a perfect heat sink. The node density (nodes per micron) is defined independently in each direction. The Y-direction also includes a sub region which can modeled with a separate density of nodes. This sub region was intended to encompass the region near thin films, where the node density in the Y-direction would need to be much higher than for the rest of the material. This subregion can be defined anywhere within (including exactly at) the overall Y_{min} and Y_{max} boundaries.

A.3 Device Layout

The HEAT program uses a group of three dimensional rectangular regions to define the geometrical and material layout of the mass being modeled. These regions are referred to as "elements," and are defined in space with X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, and Z_{max} coordinates. These values must be contained between, or on the overall grid boundary coordinates. These element boundary coordinates can be assigned arbitrarily within these bounds, and do not need to be located at a node coordinate. Each element generally contains many nodes, and is made up of a single material. Each element exhibits the properties associated with that material.

A.4 Power Distribution

HEAT versions 1.0 to 3.3 assume that power is distributed iniformly over a sub group of elements. In the configuration file, each element is designated as either passive or active. The total input power is distributed evenly among the active elements. The power input for an individual node is calulated according to the following formula:

$$\text{Power at node i} = \text{Total power} \cdot \frac{\text{volume of node i}}{\text{total volume of the active elements}} \qquad \text{(A.1)}$$

A.5 Configuration Files

The HEAT program uses a configuration file for setting the parameters to be used for each thermal analysis. Configuration files can have any name and can be edited with any text editor. The "EDIT" program that comes with MS-DOS versions 5.0 and later is useful for this purpose. Although a configuration file can be written from scratch, it is usually much easier to modify an existing file. The HEAT program can create a default configuration file for this purpose. To create a default file, first type "HEAT" at the DOS prompt to run the program. A printout of the opening screen

is included on one of the following pages of this text. Press "S" to save the default configuration file. The program will ask for the name to be used for this configuration file. Type in the name and press <ENTER>. Raw data files can also be used as configuration files. Just type the name of the data file, and the configuration information will be read from the file. Type "Q" at the opening menu to quit the program.

A printout of a configuration file is listed on one of the following pages. The first line is the file header. Do not delete or change this line. The next line states how many elements will be listed in the element list. Do not change the label to the left of the number. The HEAT program looks for "# OF ELEMENTS USED", and then inputs the number at the end of this line. The distance from the label is unimportant, and can be changed. The rest of the input file is edited in this manner.

A "THERMAL CONDUCTIVITY" line should exist for each material used. The number of these lines should match the number at the end of the "# OF MATERIALS" line. The heat capacity data is ignored for steady state analysis, and can be deleted if this is the case.

Each element is defined by eight lines, beginning with "MATERIAL NUMBER" and ending with "DISSIPATED ...". Spaces can be inserted between each element group. A remark line can be inserted to help with the bookkeeping. The HEAT program will usually ignore any blank lines, or any line in which it doesn't recogize the label, but use an apostrophe or a "REM" at the beginning of the comment lines to help avoid confusing the HEAT program (see example).

Never put a space between a minus sign and a digit.

Always leave the "END FILE" label at the end of the file.

A.6 Running the Program

Start the program by typing "HEAT" at the DOS prompt. The right part will list which commands are available. The left part of the screen will show a graphical representation of the default configuration. To load a new configuration file, type "L". It is suggested that the **View Config** command (press "V") be used to verify that the

correct information was read from the configuration file. The left side of screen will show an X-Y cross section at Z=0 to help verify the configuration file.

Press "D" to load a raw data file. The program will ask for a data file name.

Typing "C" will cause the program to first ask how many iteration loops to calculate before it stops, and then it will start computing. The node to node impedances are first computed, and then the iteration loops are performed. The program will continue computing until either the specified number of loops are completed, or until the "X" button is pressed. Once the iterations are stopped, the second menu screen appears which displays all the available commands. At this point, you probably should save the data by pressing the "S" button.

Pressing "1" though "6" calls each of the available thermal plotting routines for viewing the thermal data. Each of these routines also allows a subset of the raw data to be saved in a tab-delineated file format (cricket graph format) for manipulation with outside programs. Once inside a plotting routine, the "1" and "2" buttons are used to activate cursor buttons which can be used to accurately read data point positions or slopes.

Type "C" to continue with more iteration loops. The impedance values are recalculated at this time because they are erased when the iterations are stopped, to allow memory allocation for the plotting routines. This was done to maximize the memory available for the iterations.

The only way to get back to the first menu is by pressing the <Esc> key. Doing this erases the raw thermal data from memory.

The RAMDISK location is the path for the temporary files that are created when isothermal plots ares saved as files to the disk. If available, it is suggested that a ram disk be used for this function, although any avalible disk space will work. If the RAMDISK location is left blank, then the temporary filles are created and erased from the current path. The RAMDISK location can be changed by pressing "R".

A.7 Running Batch commands

A series of simulations can be run unattended using the RUN BATCH FILE feature of the HEAT program. By pressing "B" from the opening menu, HEAT will begin simulations based on configuration files listed in a text file named "HEAT.RUN". An example of HEAT.RUN is listed below.

```
TEST1.CFG, TEST1.DAT, 1E-4, 20000
TEST2.CFG, TEST2.DAT, 1E-4, 20000
```

Each line corresponds to one simulation. The first item in each line is the name of the configuration file. The second item is the name of the raw data file that is to be used to save the data. The third and fourth items are conditions for stopping the iteration loops for each simulation. The third item is the minimum allowable percent change in temperature of the system per iteration loop. The formula used to calculate this value is given as:

$$\text{Minimum\% temperature increment} = \frac{\text{maximum temperature change}}{\text{maximum temperature of the system}} \div 100 \qquad \text{(A.2)}$$

The simulation will be stopped if this number falls below the number listed as the third item. The last item in each line is the maximum number of iteration loops that HEAT will perform for that simulation. A simulation is finished when either of the two conditions is met.

An example of a configuration file is shown on the next two pages.

Example Configuration File for the HEAT Program

```
HEAT CONFIGURATION FILE
# OF ELEMENTS USED              3
# OF MATERIALS IN LIST          3
TOTAL POWER DISSIPATED          .000001
# ITERATION LOOPS COMPLETED     0
MINIMUM X COORDINATE (microns)  0
MAXIMUM X COORDINATE (microns)  5
MINIMUM HI-RES Y     (microns) -1
MAXIMUM HI-RES Y     (microns)  .5
MINIMUM LO-RES Y     (microns) -5
MAXIMUM LO-RES Y     (microns)  .5
MINIMUM Z COORDINATE (microns)  0
MAXIMUM Z COORDINATE (microns)  5
NODES/MICRON  X          1
NODES/MICRON  Z          1
NODES/MICRON  HI-RES Y   6
NODES/MICRON  LO-RES Y   2

*** TRANSIENT ANALYSIS OPTIONS ******
TIME CONSTANT (seconds)   .001
STEADY STATE or TRANSIENT (1=STEADY STATE); 2=TRANSIENT  1

*********** DEFAULT BOUNDARY CONDITIONS ***************
    1   : INSULATOR
    2   : THERMAL SINK
 @ X < Xmin  : BOUNDARY CONDITION   1
 @ X > Xmax  : BOUNDARY CONDITION   2
 @ Y < Ymin  : BOUNDARY CONDITION   2
 @ Y > Ymax  : BOUNDARY CONDITION   1
 @ Z < Zmin  : BOUNDARY CONDITION   1
 @ Z > Zmax  : BOUNDARY CONDITION   2

++++ MATERIAL DATA ++++++++++++
THERMAL CONDUCTIVITY  (W/cm/K)   .027
THERMAL CONDUCTIVITY  (W/cm/K)   .018
THERMAL CONDUCTIVITY  (W/cm/K)   3.15

*** HEAT CAPACITY VALUES ARE IGNORED FOR STEADY STATE
ANALYSIS **
HEAT CAPACITY (W*sec/cm^3)   1
HEAT CAPACITY (W*sec/cm^3)   1
HEAT CAPACITY (W*sec/cm^3)   1
```

(The example configuration file is continued on the next page.)

```
^^^^^^^^^ ELEMENT DATA ^^^^^^^^^^^^^^
'** BISMUTH HEATER ELEMENT ***
MATERIAL NUMBER  1
Xmin   0
Ymin   0
Zmin   0
Xmax   2
Ymax   .25
Zmax   2
DISSIPATED POWER IN THIS ELEMENT (0=NO; 1=YES)  1

'-- QUARTZ SUBSTATE ----
MATERIAL NUMBER  2
Xmin   0
Ymin  -5
Zmin   0
Xmax   5
Ymax   0
Zmax   5
DISSIPATED POWER IN THIS ELEMENT (0=NO; 1=YES)  0

REM ** gold antenna leads **
MATERIAL NUMBER  3
Xmin   2
Ymin   0
Zmin   0
Xmax   5
Ymax   .5
Zmax   2
DISSIPATED POWER IN THIS ELEMENT (0=NO; 1=YES)  0

END FILE
```

Appendix B

The following formula was adapted from *Numerical Recipes, The Art of Scientific Computing*, by W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling; Cambridge University press, 1986, page 164

```
FUNCTION ERFC (z)
'THIS ROUTINE CALCULATES THE COMPLIMENTARY ERROR FUNCTION USING THE
'ALGORITHM GIVEN IN "NUMERICAL RECIPES"
'FRACTION ERROR EVERYWHERE IS LESS THAN 1.2E-7

 T = 1 / (1 + .5 * z)
 middle = T * (.27886807# + T * (-1.13520398# + T * (1.48851587# + T
* (-.82215223# + T * .17087277#))))
 erffc = T * EXP(-z * z - 1.26551223# + T * (1.00002368# + T *
(.37409196# + T * (.09678418# + T * (-.18628806# + middle)))))
 IF erffc > 1 THEN erffc = 1
ERFC = erffc
END FUNCTION
```

Appendix C

Appendix C details the solution of

$$Q(x,\tau) = \int_0^{\tau} q(x,t)dt \tag{C.1}$$

where

$$q(x,t) = q_o \cdot \operatorname{erfc}\left(\frac{x}{2 \cdot \alpha^{1/2} \cdot t^{1/2}}\right) \tag{C.2}$$

Begin by making the substitutions

$$\operatorname{erfc}(Z) = 1 - \operatorname{erf}(Z) \tag{C.3}$$

$$A = \frac{x}{2 \cdot \alpha^{1/2}} \tag{C.4}$$

$$\therefore Q(x,\tau) = q_o \cdot \tau - q_o \int_0^{\tau} \operatorname{erf}\left(A \cdot t^{-1/2}\right)dt \tag{C.5}$$

The problem is now reduced to solving

$$\int_o^{\tau} \operatorname{erf}\left(A \cdot t^{-1/2}\right)dt \tag{C.6}$$

Begin solving this by using the identity given in chapter 3 (equation 3.36) and integration by parts, where

$$U = \operatorname{erf}\left(A \cdot t^{-1/2}\right) \qquad dV = dt \tag{C.7}$$

$$dU = -A \cdot \pi^{-1/2} \cdot t^{-3/2} \cdot \exp\left(-A^2 \cdot t^{-1}\right) \qquad V = t \tag{C.8}$$

$$\int U \cdot dV = U \cdot V - \int V \cdot du \tag{C.9}$$

to produce

$$\int_0^{\tau} \operatorname{erf}\left(A \cdot t^{-1/2}\right) dt = \tau \cdot \operatorname{erf}\left(A \cdot \tau^{-1/2}\right) + \frac{A}{\pi^{1/2}} \cdot \int_0^{\tau} t^{-1/2} \cdot \exp\left(-A^2 \cdot t^{-1}\right) dt \qquad \text{(C.10)}$$

By repeating integration by parts on the right term, in which

$$dV = t^{-1/2}, t^{-3/2}, t^{-5/2}, t^{-7/2}, \text{etc...}$$

for each sucessive integration, this term can be represented as

(C.11)

$$\int_0^{\tau} t^{-1/2} \cdot e^{-\left(A^2 \cdot t^{-1}\right)} dt =$$

$$\left\{ 2 \cdot t^{1/2} \cdot e^{-\left(A^2 \cdot t^{-1}\right)} + 4 \cdot A \cdot e^{-\left(A^2 \cdot t^{-1}\right)} \cdot \sum_{n=0}^{\infty} \frac{2^n}{1 \cdot 3 \cdot (2 \cdot n)} \cdot \left(\frac{A}{t^{1/2}} \right)^{2 \cdot n + 1} \right\} \Bigg|_{t=0}^{t=\tau}$$

By using the identity

$$\operatorname{erf}(Z) = \frac{2}{\pi^{1/2}} \cdot e^{-\left(Z^2\right)} \cdot \sum_{n=0}^{\infty} \frac{2^n}{1 \cdot 3 \cdot (2 \cdot n + 1)} \cdot Z^{2 \cdot n + 1} \qquad \text{(C.12)}$$

M. Abrahmowitz and I. A. Steggum (ed.), *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables,* US Department of Commerce, National Bureau of Standards, Applied Mathematics Series, 1972. Page 297, equation 7.16.

Equation C.11 can be reduced to

(C.13)

$$\int_0^{\tau} t^{-1/2} \cdot e^{-\left(A^2 \cdot t^{-1}\right)} dt = \left\{ 2 \cdot t^{1/2} \cdot e^{-\left(A^2 \cdot t^{-1}\right)} + 2 \cdot \pi^{1/2} \cdot A \cdot \operatorname{erf}\left(A \cdot t^{1/2}\right) \right\} \Bigg|_{t=0}^{t=\tau}$$

Solving for the limits of integration gives

(C.14)

$$\therefore \int_0^{\tau} t^{-1/2} \cdot e^{-\left(A^2 \cdot t^{-1}\right)} dt = 2 \cdot \tau^{1/2} \cdot e^{-\left(A^2 \cdot \tau^{-1}\right)} + 2 \cdot \pi^{1/2} \cdot A \cdot \left[\operatorname{erf}\left(A \cdot \tau^{-1/2} \right) - 1 \right]$$

Substituting equation C.14 into far right term in equation C.10 produces

(C.15)

$$\int_0^{\tau} \operatorname{erf}\left(A \cdot t^{-1/2} \right) dt = \tau \cdot \operatorname{erf}\left(A \cdot \tau^{-1/2} \right) + \frac{2}{\pi^{1/2}} \cdot A \cdot \tau^{1/2} \cdot e^{-\left(A^2 \cdot \tau^{-1}\right)} + 2 \cdot A^2 \cdot \operatorname{erf}\left(A \cdot \tau^{-1/2} \right) - 2 \cdot A^2$$

Equation C.15 can be checked by taking the derivative of both sides of the equation and making sure that they match. The derivative of the error function is given in equation 3.36 (see chapter 3).

We now have the solution to equation C.6. This solution can be substituted into equation C.5 to get a new expression for equation C.1.

$$Q(x,\tau) = q_o \cdot \left\{ \left(\tau + \frac{x^2}{2 \cdot \alpha} \right) \cdot \operatorname{erfc}\left(\frac{x}{2 \cdot \alpha^{1/2} \cdot \tau^{1/2}} \right) - \frac{x \cdot \tau^{1/2}}{\alpha^{1/2} \cdot \pi^{1/2}} \cdot \exp\left(\frac{-x^2}{4 \cdot \alpha \cdot \tau} \right) \right\} \quad \text{(C.16)}$$

Appendix D

Detector Layer Lithographic Step

This section details the lithographic process for patterning the first layer (YBCO) for the HiTc microbolometers in this study. The plasma process in step 1 uses a March Instruments research sized barrel reactor. The etchant recipe using ethylenedinitrilotetraacetic acid (EDTA) was supplied by Alan Berezin (Department of Physics, University of Texas at Austin). The photoresist baking steps were done by placing the chip on a hot aluminum block (~5 cm x ~5 cm x ~1 cm) inside an oven.

1. **Prepare the film surface** with an oxygen plasma at ~ 600 militorr, 1/2 power, for 2 minutes.
2. **Spin on** AZ 1350J resist for 30 seconds at 550 rpm.
3. **Soft bake** 75 seconds on a hot block in a 90 °C oven.
4. **Expose** the edge bead mask 65 seconds at 8.1 mW/cm^2.
5. **Develop** 45 seconds using 452 deveoper.
6. **Expose** "combo II" mask
7. **Develop** 45 seconds.
8. **Examine** the substrate under a microscope to verify the resist pattern before etching.
9. **Prepare** etchant by mixing ~ teaspoon of EDTA powder into ~ 100 ml of de-ionized water. Add more powder if necessary to make a saturated solution with small amount of undissolved powder at the bottom of the beaker. Let the solution stand for few minutes.
10. **Etch** the sample in the EDTA solution for about 30 seconds. The etching rate seemed to vary with different samples.
11. **Rinse** in de-ionized water and blow dry with dry nitrogen.
12. **Examine** the film under a microscope to check the etch pattern. Etch more if necessary.
13. **Remove** "scum" from the substrate surface where the YBCO has been etched away by lightly scrubbing with several wet Q-tips. The resist is left on for this step to protect the underlying device, and to keep the scum from being smeared onto the remaining YBCO material.
14. **Strip resist** in acetone ~ 60 seconds.
15. **Rinse** in ethanol, followed by de-ionized water.

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