MARTIN MARIETTA ENERGY SYSTEMS LIBRARIES

3 4456 0334900 8

ORNL/TM-11734

ornl

OAK RIDGE
NATIONAL
LABORATORY

MARTIN MARIETTA

Casting of HgCdTe Part 1: Thermophysical Property Values

V. Alexiades

OAK RIDGE NATIONAL LABORATORY
CENTRAL RESEARCH LIBRARY
CIRCULATION SECTION
4500N ROOM 175
LIBRARY LOAN COPY
DO NOT TRANSFER TO ANOTHER PERSON
If you wish someone else to see this report, send in name with report and the library will arrange a loan.

MANAGED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831; prices available from (615) 576-8401, FTS 626-8401.

Available to the public from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161.

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ORNL/TM-11734

Engineering Physics and Mathematics Division
Mathematical Sciences Section

CASTING OF HgCdTe

Part I: Thermophysical Property Values

Vasilios Alexiades

Mathematical Sciences Section
Engineering Physics and Mathematics Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-8083
and
Mathematics Department
University of Tennessee
Knoxville, TN 37996-1300

Date Published: March 1991

Research supported by the Microgravity Science and Applications Division of NASA under contract H-80582B with the Oak Ridge National Laboratory; and by the Science Alliance, a Centers of Excellence Program of the State of Tennessee at the University of Tennessee, Knoxville.

Prepared by the
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
Managed By
MARTIN MARIETTA ENERGY SYSTEMS, INC.
for the
U.S. DEPARTMENT OF ENERGY
under Contract No. DE-AC05-840R21400

MARTIN MARIETTA ENERGY SYSTEMS LIBRARIES

3 4456 0334900 8

TABLE OF CONTENTS

Abstract 1

1. Introduction 1

2. Phase Diagram 3

3. Specific Heats 5

3.A Specific Heat of Liquid, $c_P^L(x, T)$ 5

3.B Specific Heat of Liquid $HgTe$, $c_{P,AC}^L(T)$ 5

3.C Specific Heat of Solid, $c_P^S(x, T)$ 9

4. Partial Enthalpies 9

4.A Partial Specific Enthalpy Difference for Liquid 9

4.B Specific Partial Enthalpy Difference for Solid 11

5. Densities 13

5.A Density of Liquid, $\rho^L(x, T)$ 13

5.B Density of Solid, $\rho^S(x, T)$ 13

6. Thermal Conductivities 13

6.A Thermal Conductivity of Liquid, $k^L(x, T)$ 14

6.B Thermal Conductivity of Solid, $k^S(x, T)$ 14

7. Solute Diffusivities, D^L, D^S 14

References 17

CASTING OF HgCdTe

Part I: Thermophysical Property Values

Vasilios Alexiades

Mathematics Department
University of Tennessee
Knoxville, Tennessee 37996-1300

and

Mathematical Sciences Section
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-8083

ABSTRACT

Mercury-Cadmium-Telluride is a technologically important electronic material, used primarily as an infrared-detector. In such applications, large crystals of uniform concentration are desirable, which is difficult to achieve when the crystal is grown under gravity. Modeling and numerical simulation can help us gain insight, in the interpretation of experiments, and in designing future earth-bound and microgravity experiments.

In this report we present a compilation of the relevant thermophysical properties of the pseudo-binary $(HgTe)_{1-x}(CdTe)_x$, as functions of composition, x, and temperature, for both the solid and liquid phases, at the high temperatures ($\approx 600-1100°C$) relevant in the casting process. We compile those properties which are needed in our solidification model and numerical code presented in [1]. In addition to the liquidus and solidus curves of the phase diagram, these include: densities, heat capacities, partial enthalpies, thermal conductivities and solute diffusivities. They are presented in the form of formulas, easy to evaluate, obtained by curve-fitting available data.

1. INTRODUCTION

Mercury-Cadmium-Telluride is a versatile infrared-detector alloy for which large crystals of uniform composition are desirable. This is very difficult to achieve in any of the bulk crystal growth methods used for its prepartion, see Nelson-Higgins-Lancaster [5] for a review. A better quantitative understanding of the solidification process is necessary in order to know how the various parameters of the process effect the final composition.

Modeling and numerical simulation can help us gain such insight, as well as help in interpreting experimental measurements and in designing future earth-bound and microgravity experiments. In support of an ongoing experimental program at NASA/Huntsville, we have undertaken the modeling and simulation of the casting process used in the preparation of the alloy.

The models require values of the thermophysical properties of the alloy as input parameters, so in this first report we present a compilation of the relevant properties. In addition to the liquidus and solidus curves of the phase-diagram, these include: **densities, heat capacities, partial enthalpies, thermal conductivities** and **solute diffusivities** for both the *solid and liquid phases*, as functions of *composition*, x, and *temperature*, T, of the pseudo-binary

$$(HgTe)_{1-x}(CdTe)_x \ .$$

The range of temperatures relevant for the casting process is roughly 600–1100°C. Such high temperatures make direct experimental measurements difficult, so few of the properties have been measured directly, [2-9].

Fortunately, good thermodynamical models have been developed for both the solid and liquid phases [2], [10], from which we can obtain needed property values (see §2,3,4).

It is convenient for computational purposes (and necessary for efficiency) to have simple expressions for all the thermophysical properties, so that, given x and T, the desired value can be found by a simple evaluation. This report presents a list of such formulae, compiled by least-squares-fitting of property values to as simple expressions as we could generate to within an error of about 1%.

The basic thermophysical properties discussed are:

- Liquidus and Solidus curves of the phase-diagram: $x = x^L(T)$, $x = x^S(T)$;
- heat capacities: $c_P^L(x,T)$, $c_P^S(x,T)$;
- partial enthalpies: $\bar{h}^L(x,T)$, $\bar{h}^S(x,T)$;
- densities: $\rho^L(x,T)$, $\rho^S(x,T)$;
- thermal conductivities: $k^L(x,T)$, $k^S(x,T)$;
- solute diffusivities: $D^L(x,T)$, $D^S(x,T)$.

In addition, various related quantities needed in our models will be discussed.

Concerning *units*, we will consistently use: **cm**, **g**(*gram*), **s**(*sec*), **°C**, and our final formulae will be for the *specific heats*, (in $cal/g\ °C$) *specific partial enthalpies* (in cal/g), densities (in g/cm^3), conductivities (in $cal/s\ cm\ °C$), and diffusivities (in cm^2/s). The composition variable x, is the x in the formula $(HgTe)_{1-x}(CdTe)_x$, which for convenience we will represent by the simpler symbols $(AC)_{1-x}(BC)_x$, i.e. $A = Hg, B = Cd, C = Te$. Following standard practice in the Physical Chemistry literature [10], we interpret the formula in g-atoms, meaning "per Avogardro's number". Thus **1 g-atom** of $A_{1-x}\ B_x\ C$ consists of ½(x − 1) moles of A atoms, ½x moles of B atoms, and ½ moles of C atoms. Therefore, the mass, in grams, of 1 g-atom of $A_{1-x}\ B_x\ C$ is:

$$\frac{(x-1)}{2} M_A + \frac{x}{2} M_B + \tfrac{1}{2} M_C =: \tfrac{1}{2} M(x)$$

where M_i, denotes the g-atomic weight of component $i = A, B, C$, and

$$M(x) := M_A(1-x) + M_B\, x + M_C \tag{1.1}$$

is the gram-formula weight (also commonly called molecular weight). For us, $M_A \equiv M_{Hg} = 200.6, M_B \equiv M_{Cd} = 112.4, M_C \equiv M_{Te} = 127.6$, so

$$M(x) = 328.2(1-x) + 240.0\,x \equiv 328.2 - 88.2\,x, \quad 0 \le x \le 1, \tag{1.2}$$

and the conversion factor from "per g-atom" to "per gram" is $\frac{2}{M(x)}$.

2. PHASE DIAGRAM

The phase diagram of the pseudobinary $(HgTe)_{1-x}(CdTe)_x$ is discussed in [11], [12], [9]. The most complete data are from the book chapter by Brebrick-Su-Liao [2], shown in **Table 2.1**. These values are consistent with an associated solution model for the liquid phase and a quasiregular solution model for the solid phase, developed in [2]. These same models will be used in §3 and §4 also, resulting in property values thermodynamically consistent with the phase-diagram. Such consistency is important, at least conceptually, for our solidification model which will be presented in [1].

TABLE 2.1 Solidus and Liquidus data from [2]

x	Solidus $T = T^S(x)$	Liquidus $T = T^L(x)$	Solidus composition $x^S(T)$ corresponding to $T = T^L$
0.0	670.0°	670.0°	0.
.1	686.2	736.0	.36
.2	703.6	792.0	.564
.3		838.0	.685
.4	745.5	879.0	.768
.5		918.0	.832
.6	803.8	955.6	.882
.7		991.0	.9233
.8	897.5	1025.0	.957
.9	969.4	1059.0	.983
.925	991.8		
.95	1018.2		
1.0	1092.0	1092.0	1.0

The first vs third columns of **Table 2.1** display 11 points for the liquidus curve $x = x^L(T)$, which we have fitted to the expressions:

$$x^L(T_0) = a_1 T_0 + a_2 T_0^{5/2} + a_3 T_0^3, \quad T_0 = \frac{T-670}{422}, \quad (T \text{ in } °C)$$

$$a_1 = 0.567785834310387$$

$$a_2 = 1.231077146918574 \tag{2.1}$$

$$a_3 = -0.7995987198265$$

with maximum relative error 0.86% and average relative error 0.55%; its inverse, $T = T^L(x)$ may be represented by

$$T^L(x) = 670 + 422 \cdot [b_1 x + b_2 x^{3/2} + b_3 x^{5/2}] \quad (T \text{ in } °C)$$

$$b_1 = 1.996705576827808 \tag{2.2}$$

$$b_2 = -1.310070463246959$$

$$b_3 = 0.314567918610010$$

with maximum relative error 0.83% and average relative error 0.47%.

Note that x^L and T^L are supposed to be inverse functions of each other, but the relation $x^L(T_0^L(x)) = x$ is only satisfied numerically to a much lower precision due to roundoff. Either one of (2.1) or (2.2) provides an excellent fit to the liquidus data, but to retain full precision one should find the inverse by solving the appropriate equation ($x^L(T_0) = x$ or $T^L(x) = T$) via a Newton-Raphson method, rather than using the corresponding fit.

For the solidus curve, $x = x^S(T)$ or $T = T^S(x)$, 15 points are available from **Table 2.1**, which we have fitted to the expressions:

$$x^S(T_0) = A_1 T_0 + A_2 T_0^2 + A_3 \ln(1 + T_0), \quad T_0 = \frac{T-670}{422}, \quad (T \text{ in } °C),$$

$$A_1 = -6.699411637535547 \tag{2.3}$$

$$A_2 = 1.141303649411918$$

$$A_3 = 9.470191809366767$$

with maximum relative error 0.43% and average relative error 0.41%; and

$$T^S(x) = 670 + 422\,[B_1(2x^2 - 1) + B_2 \cos x + B_3 e^{2x^2 - 1} + B_4 \ln(1 + x) + B_5(e^x - 1)] \quad (°C)$$

$$B_1 = 7.51007039423875 \qquad B_4 = 12.334324484013730 \tag{2.4}$$

$$B_2 = 7.306891966418074 \qquad B_5 = -11.949181192924680$$

$$B_3 = 0.556367799165661$$

with maximum relative error 1.22% and average relative error 0.79%. Despite an extensive search, we couldn't find a better looking fit to the solidus temperature! All simpler expressions we tried had negative slope near $x = 0$ and were rejected. Thus, it is better to represent the solidus by (2.3) and then find its inverse via Newton-Raphson to machine precision, whenever the latter is needed.

The curves (2.1) and (2.3) are plotted in **Figure 2.1**.

3. SPECIFIC HEATS

No direct experimental measurements of the heat capacities of *HgCdTe* exist. This has prompted C.-H. Su [10] to calculate them directly from the thermodynamic models for the melt and the solid developed in [2].

3.A Specific Heat of Liquid, $c_P^L(x, T)$

Values for the integral heat capacity $C_P^L(x, T)$, in cal/g-atom K, have been produced by C.-H. Su [10]. To convert to $cal/g\ K$, we divide by $\frac{1}{2}M(x) \equiv$ weight of a g-atom of components, see (1.1). The resulting values of the **specific heat of liquid** were fitted to the expression

$$c_P^L(x,T) = \{C_1 x + C_2 x + C_3 x^3\} + \{C_4 + C_5 x + C_6 x^2 + C_7 x^3\}\frac{T}{10^3} + \{C_8 + C_9 x\}(\frac{10^3}{T})^2,$$

$$(cal/g\ °C),\quad 0 \le x \le 1,\quad T > T^L(x) \tag{3.1}$$

$$\begin{array}{ll} C_1 = -0.16025 & C_6 = -0.297 \\ C_2 = 0.46369 & C_7 = 0.450327 \\ C_3 = -0.60127 & C_8 = 0.01056 \\ C_4 = 0.0342575 & C_9 = 0.10229 \\ C_5 = 0.0661 & \end{array}$$

with *maximum* relative error 1.9% and *average* relative error 0.6%. **Figure 3.1** shows the temperature dependence of c_P^L at compositions $x = 0, 0.1, \ldots, 1$, calculated from (3.1).

3.B Specific Heat of Liquid HgTe, $c_{P,AC}^L(T)$

In our solidification model we shall use integrations of the specific heat $c_{P,AC}^L(T)$ of $AC = HgTe$ repeatly, so we consider it prudent to employ a better approximation than the one obtained from (3.1) for $x = 0$. Such an expression is

$$c_{P,AC}^L(T) = D_1 + D_2\frac{10^3}{T} + D_3(\frac{10^3}{T})^2, \quad (cal/g\,°C) \tag{3.2}$$

$$D_1 = 0.085101608837466,\quad D_2 = -0.069850198915,\quad D_3 = 0.029490481686328$$

with *maximum* relative error 0.95% and *average* relative error 0.5%. It is plotted in **Figure 3.2**.

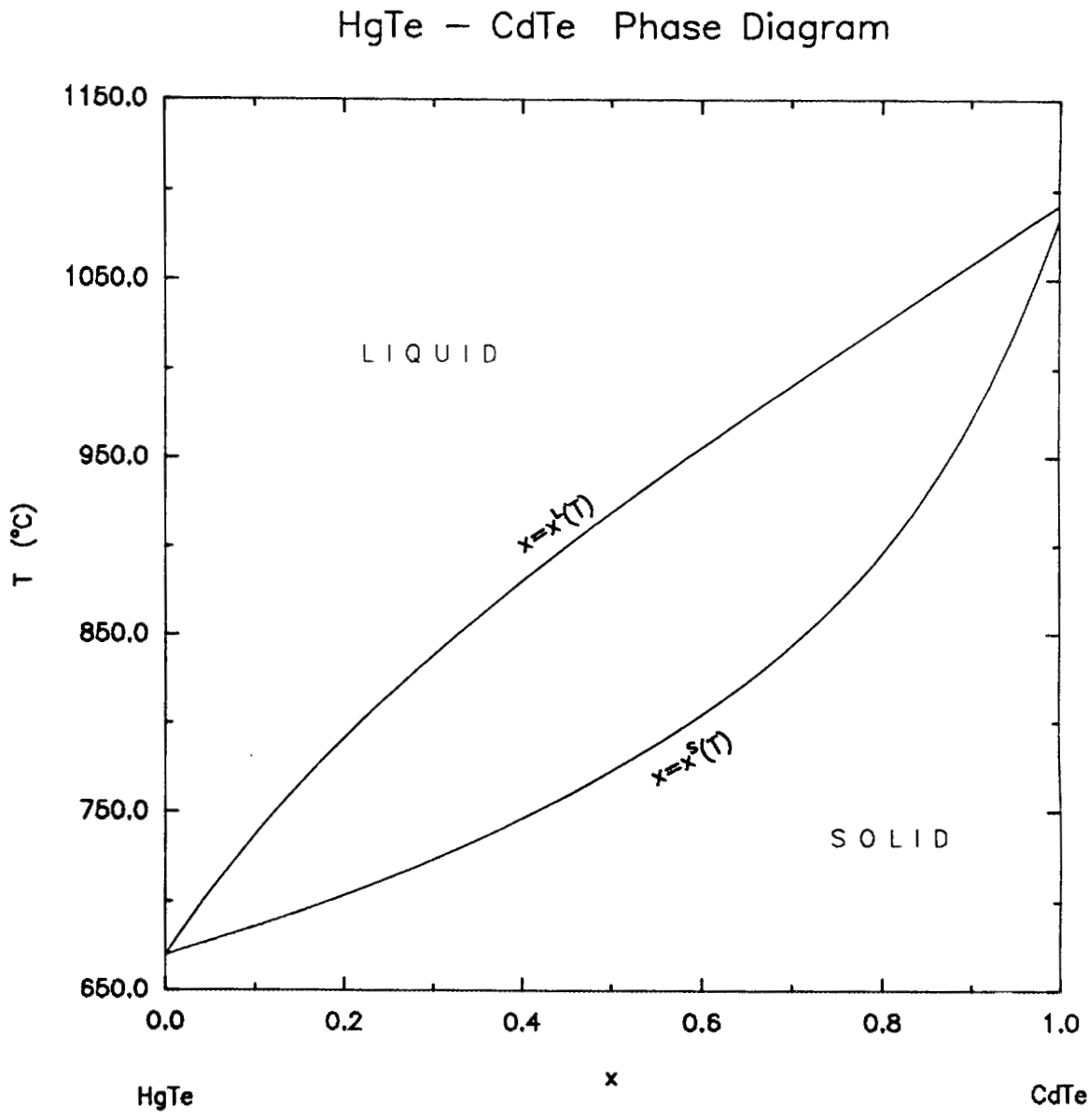
HgTe – CdTe Phase Diagram
1150.0
1050.0
950.0
850.0
750.0
650.0
T (°C)
LIQUID
SOLID
x=x^L(T)
x=x^S(T)
0.0
0.2
0.4
0.6
0.8
1.0
x
HgTe
CdTe

Figure 2.1

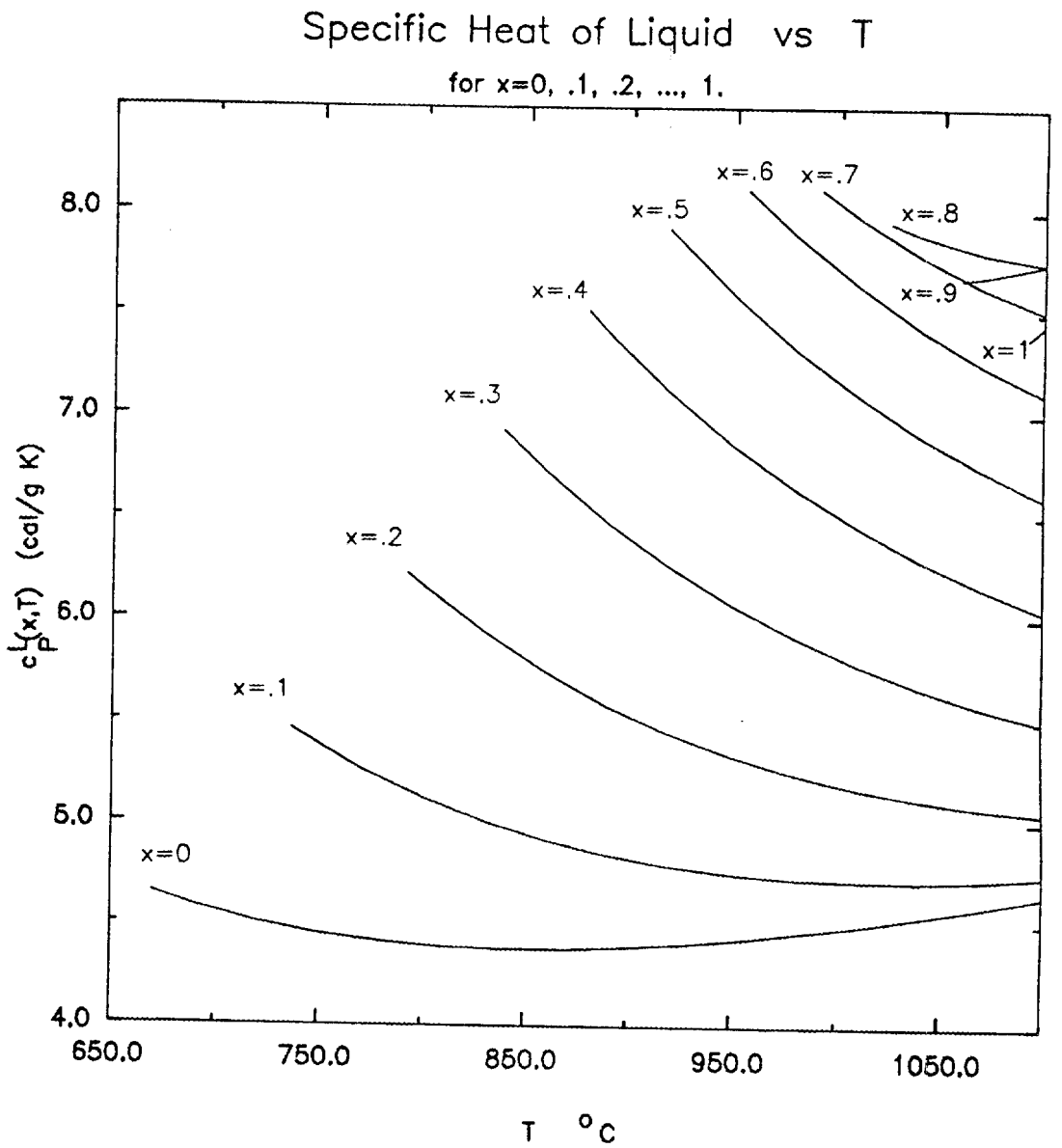
Specific Heat of Liquid vs T
for x=0, .1, .2, ..., 1.
x=0
x=.1
x=.2
x=.3
x=.4
x=.5
x=.6
x=.7
x=.8
x=.9
x=1
8.0
7.0
6.0
5.0
4.0
650.0
750.0
850.0
950.0
1050.0
T °C
$c_p^L(x,T)$ (cal/g K)

Figure 3.1

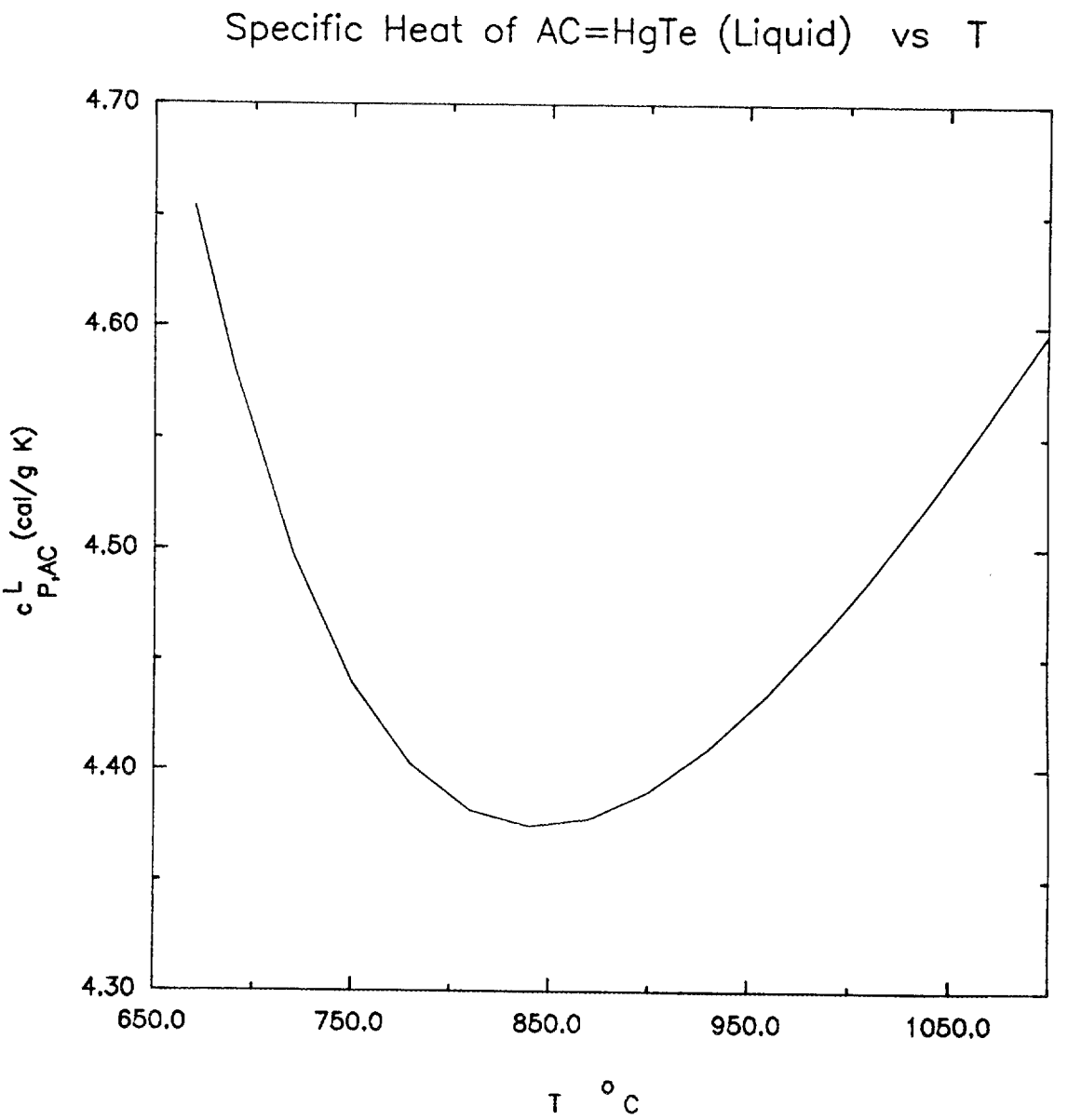
Specific Heat of AC=HgTe (Liquid) vs T
4.70
4.60
4.50
4.40
4.30
$c^L_{P,AC}$ (cal/g K)
650.0
750.0
850.0
950.0
1050.0
T °C

Figure 3.2

3.C Specific Heat of Solid, $c_P^S(x, T)$

A "quasiregular solution model" for the solid phase has been shown to be satisfactory [9], [10]. Consequently, the integral heat capacity is given by

$$C_P^S(x,T) = (1-x)C_{P,HgTe}^S(T) + C_{P,CdTe}^S(T) \qquad (cal/g\text{-}atom\ K)\,, \tag{3.3}$$

and expressions for the heat capacities of $HgTe$ and $CdTe$ are known from Mills [7], see Su [10]. Dividing by $\frac{1}{2}M(x)$, the resulting expression for the **specific heat of solid** may be written in the form

$$c_P^S(x,T) = \{13.042736 - 1.3148505\,x + (2.17 + 5.73\,x)\frac{T°C}{10^3}\}/M(x) \qquad (cal/g\,°C)\,, \tag{3.4}$$

with $M(x)$ as in (1.2). Representative plots are shown in **Figure 3.3**.

4. PARTIAL ENTHALPIES

The partial *molar* enthalpies $\overline{H}_{AC}$ and $\overline{H}_{BC}$, for either phase, as functions of composition, x, and temperature, T, can be obtained from the thermodynamic model of the pseudobinary $(AC)_{1-x}(BC)_x$, described in [2], [10]. This requires considerable computation for each (x, T), so we have fitted the values to convenient expressions, for those quantities needed in our solidification model.

4.A Partial Specific Enthalpy Difference for Liquid

We have implemented the associated solution model of Brebrick-Su-Liao [2] for liquid in a computer code. For each given (x, T), a cubic equation is solved (using the C02AEF routine of the NAG Library) and we compute the partial *molar* enthalpies $\overline{H}_{AC}^L(x,T)$ and $\overline{H}_{BC}^L(x,T)$, in cal/mol. Then we form the difference

$$\overline{h}^L(x,T) := \frac{\overline{H}_{BC}^L(x,T)}{240.} - \frac{H_{AC}^L(x,T)}{328.2} \qquad (cal/g) \tag{4.1}$$

of the partial *specific* enthalpies, which is needed in our solidification model (see [1]). The values thus obtained we have fitted to the expression

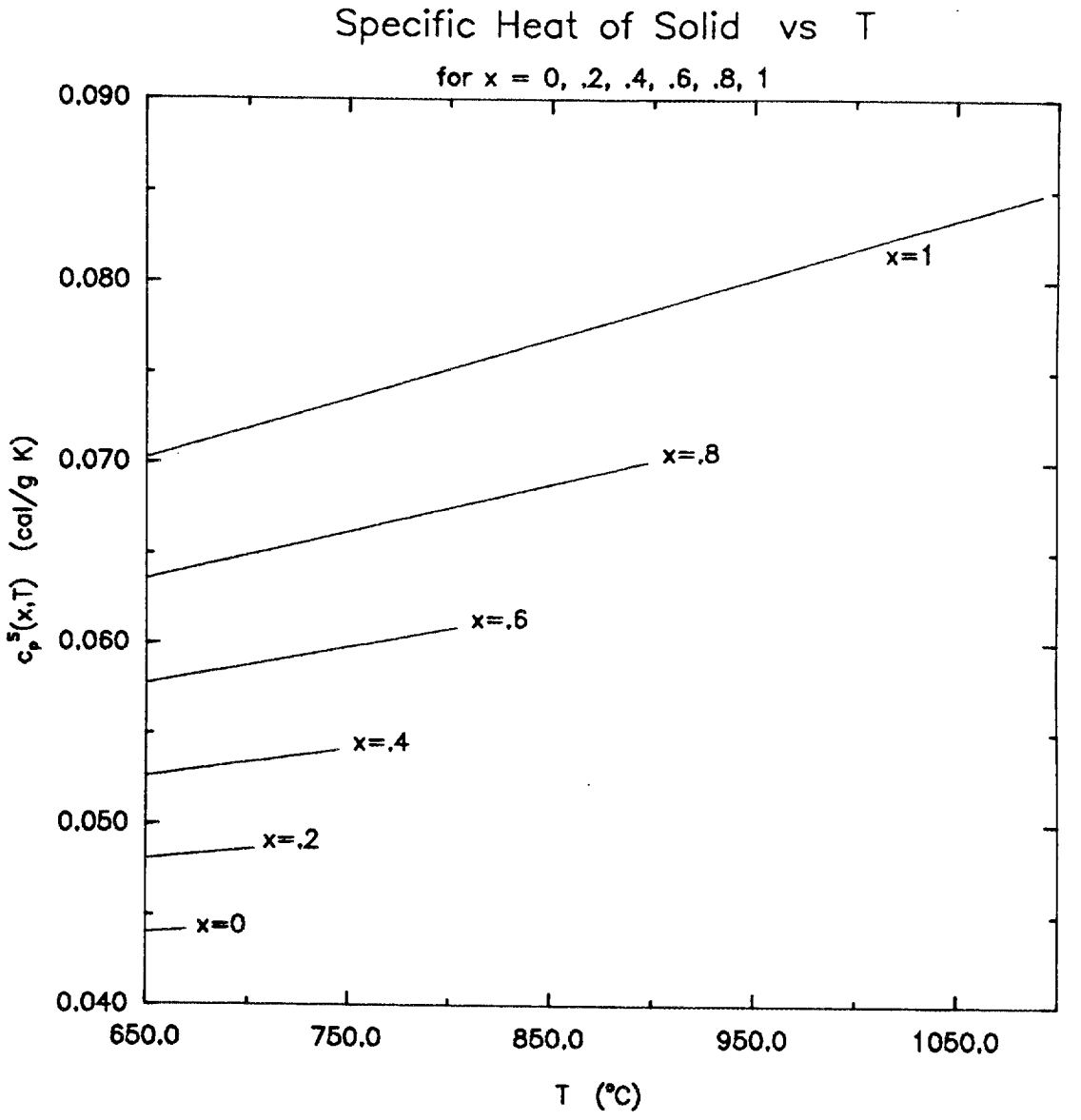
Specific Heat of Solid vs T
for x = 0, .2, .4, .6, .8, 1
0.090
0.080
0.070
0.060
0.050
0.040
$c_p^s(x,T)$ (cal/g K)
x=1
x=.8
x=.6
x=.4
x=.2
x=0
650.0
750.0
850.0
950.0
1050.0
T (°C)

Figure 3.3

$$\bar{h}^L(x,T_0) = \{E_1 + E_2 x + E_3 x^2\} + \{E_4 + E_5 x + E_6 x^2\} T_0 + E_7 T_0^2 + E_8 \sqrt{T_0} + \{E_9 + E_{10} x + E_{11} x^2\} \frac{1}{1+T_0}, \tag{4.2}$$

$$(cal/g), \quad 0 \le x \le 1, \quad T \ge T^L(x)$$

$$T_0 = (T - 670)/422 \ .$$

$E_1 = -1602.7758$	$E_7 = 359.22097913$
$E_2 = 255.4845$	$E_8 = 3620.894679$
$E_3 = 199.9833258$	$E_9 = 75.204749$
$E_4 = -2438.29341$	$E_{10} = -146.3777659$
$E_5 = -121.1964972$	$E_{11} = -94.5888894$
$E_6 = -89.30305$	

with maximum relative error 5.6% and average relative error 1.4%. Its temperature dependence is shown in **Figure 4.1** for several x values.

4.B Specific Partial Enthalpy Difference for Solid

The quasiregular solution model for the solid phase [2], leads to the following expressions for the *molar* partial enthalpies:

$$\bar{H}^S_{AC}(x,T) = \bar{H}^{0,S}_{AC}(T) + 1384\, x^2 \quad (cal/mol) \tag{4.3}$$

$$\bar{H}^S_{BC}(x,T) = \bar{H}^{0,S}_{BC}(T) + 1384(1-x)^2 \quad (cal/mol) \tag{4.4}$$

where the reference values $H^{0,S}_{AC}(T)$ and $\bar{H}^{0,S}_{BC}(T)$ (to the liquid components A, B, C) are given by

$$\bar{H}^{0,S}_{AC}(T) = -12829 - 4040.3 \left[107.1 - \frac{1122.8}{(T/10^3)} + \frac{1354.7}{(T/10^3)^2} - \frac{179.1}{(T/10^3)^3} \right] e^{-\frac{7135.68}{T}},$$

$$(cal/mol), \quad T \text{ in Kelvin}, \tag{4.5}$$

$$\bar{H}^{0,S}_{BC}(T) = -30024 \quad (cal/mol) \ . \tag{4.6}$$

Then, the difference of *specific* partial enthalpies is found to be

$$\bar{h}^S(x,T) := \frac{\bar{H}^S_{BC}}{240} - \frac{\bar{H}^S_{AC}}{328.2} = \bar{h}^{0,S}(T) - 80.241 - 11.54\, x - 9.9869\, x^2 \quad (cal/g) \tag{4.7}$$

where

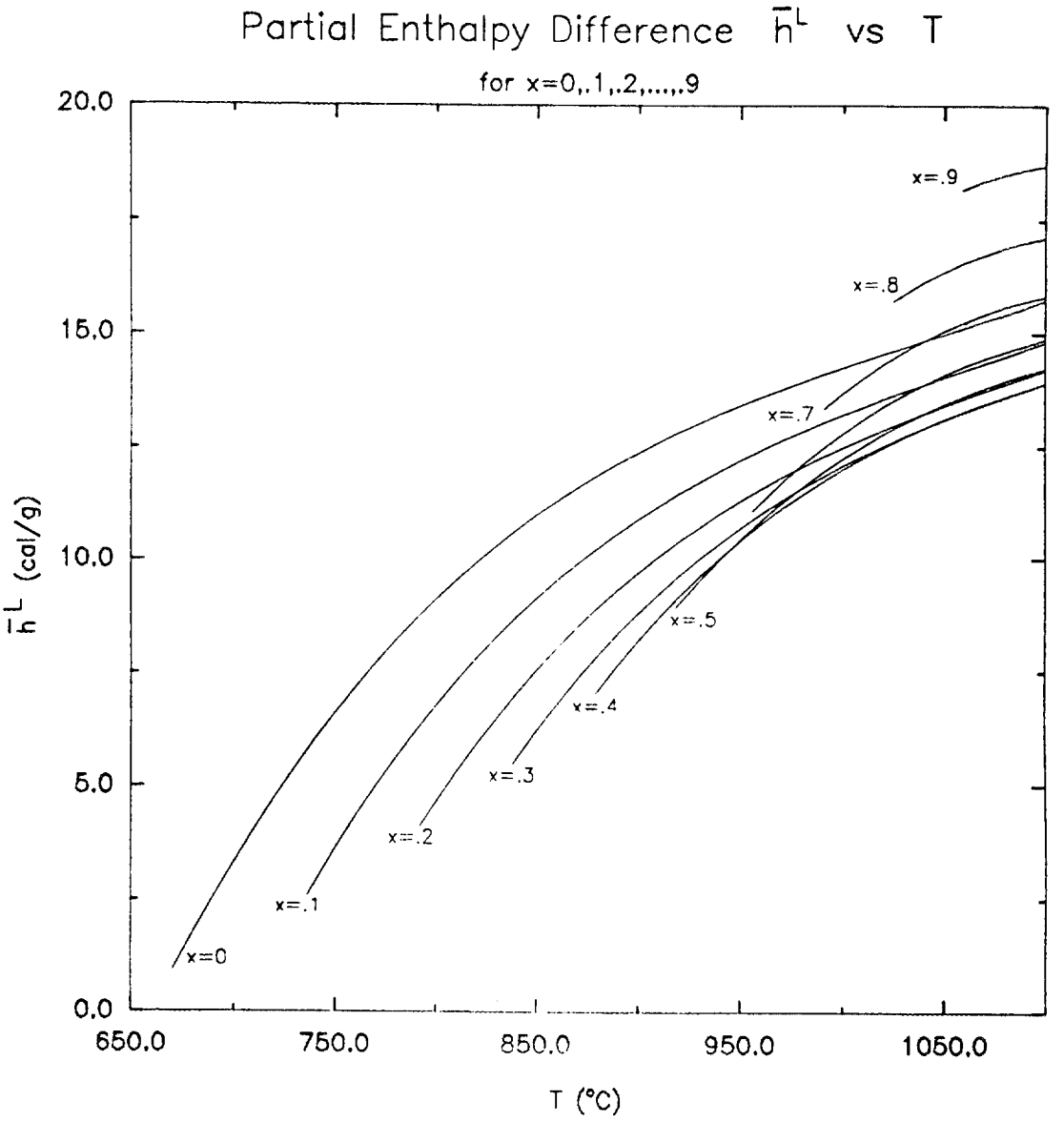
Partial Enthalpy Difference $\bar{h}^L$ vs T
for x=0,.1,.2,....,.9
20.0
15.0
10.0
5.0
0.0
650.0
750.0
850.0
950.0
1050.0
T (°C)
$\bar{h}^L$ (cal/g)
x=.9
x=.8
x=.7
x=.5
x=.4
x=.3
x=.2
x=.1
x=0

Figure 4.1

$$\bar{h}^{0,S}(T) = \left[1318.401 - \frac{13822.0373}{(T/10^3)} + \frac{16676.357}{(T/10^3)^2} - \frac{2204.721}{(T/10^3)^3} \right] e^{-\frac{7135.68}{T}} , \tag{4.8}$$

(cal/g), T in Kelvin

5. DENSITIES

5.A Density of Liquid, $\rho^L(x, T)$

The density of liquid $(HgTe)_{1-x}(CdTe)_x$ was measured by Chandra and Holland [3] in the range of $0.05 \le x \le 0.3$, $710 \le T \le 850°C$. The experimental values may be represented by the expression

$$\rho^L(x,T) = F_1 + F_2 x + \{F_3 + F_4 x\} \frac{T}{10^3} \quad (g/cm^3) \tag{5.1}$$

$F_1 = 7.897123$ $\quad F_3 = 0.18854754$
$F_2 = -0.726329$ $\quad F_4 = -2.221354$

with maximum relative error 0.23%.

5.B Density of Solid, $\rho^S(x, T)$

The density of solid solution is reported by Schwartz-Tung-Brebrick [8] as

$$\rho^S(x,T) = 8.077 - 2.225\,x \quad (g/cm^3) \ . \tag{5.2}$$

6. THERMAL CONDUCTIVITIES

There are no direct experimental measurements of thermal conductivity, see Su [10] for a discussion. We calculate them from the relationship

$$k = \rho c_P \alpha \ . \tag{6.1}$$

The only available measurements for the *thermal diffusivity*, α, are by Holland-Taylor [4], in the range $0 \le x \le 0.301$. They have curve-fitted the temperature dependence as

$$\alpha^L(x,T) = B \ln T - A \tag{6.2}$$

$$\alpha^S(x,T) = A_0 - A_1 T_* + A_2 T_*^2 - A_3 T_*^3 , \quad T_* = T/10^3 \tag{6.3}$$

and report values for the coefficients A_0, A_1, A_2, A_3, B, A at $x = 0., 0.052, 0.107, 0.205, 0.301$. Since we need the full dependence of $k(x,T) = \rho c_P \alpha$ on both x and T, we have curve-fitted the x-dependence of each of the above coefficients to expressions linear in x.

6.A Thermal Conductivity of Liquid, $k^L(x, T)$

Using (5.1), (3.1), (6.2) in (6.1), we have

$$k^L(x,T) = \rho^L(x,T)\, c_P^L(x,T)\, \alpha^L(x,T) \quad (cal/s\ cm\ °C), \tag{6.4}$$

valid, roughly, in the range $0 \le x \le 0.3$, $T \le 900°C$, where

$\rho^L(x,T)$ is given by (5.1), $c_P^L(x,T)$ is given by (3.1),
$\alpha^L(x,T)$ is given by (6.2) with

$B(x) = (9.085703 - 12.741994\,x)/100,$
$A(x) = (58.499034 - 79.4574\,x)/100.$

6.B Thermal Conductivity of Solid, $k^S(x, T)$

Using (5.2), (3.2), (6.3) in (6.1), we have

$$k^S(x,T) = \rho^S(x,T)\, c_P^S(x,T)\, \alpha^S(x,T) \quad (cal/s\ cm\ °C), \tag{6.5}$$

valid, again, for $0 \le x \le 0.3$, where

$\rho^S(x,T)$ is given by (5.2), $c_P^S(x,T)$ is given by (3.2),
$\alpha^S(x,T)$ is given by (6.3) with

$A_0(x) = (2.305915 - 5.050485\,x)/100,$
$A_1(x) = (8.33024 - 14.938646\,x)/100,$
$A_2(x) = (17.472562 - 24.771145\,x)/100,$
$A_3(x) = (13.068309 - 17.96172\,x)/100,$

The temperature dependence of the thermal diffusivities and conductivities is shown in **Figures 6.1** and **6.2** respectively, in the range $650 \le T \le 900°C$, for $x = 0, 0.1, 0.2, 0.3$.

7. SOLUTE DIFFUSIVITIES, D^L, D^S

Lehoczky-Szofran-Martin [6] report the approximate value

$$D^L = 5.5 \times 10^{-5} \quad (cm^2/s) \tag{7.1}$$

for the interdiffusion coefficient in the melt. No other data have been found.

For the solid phase, Zanio-Massopust [13] have determined the interdiffusion coefficient in the range $400°C$ to $600°C$ to be

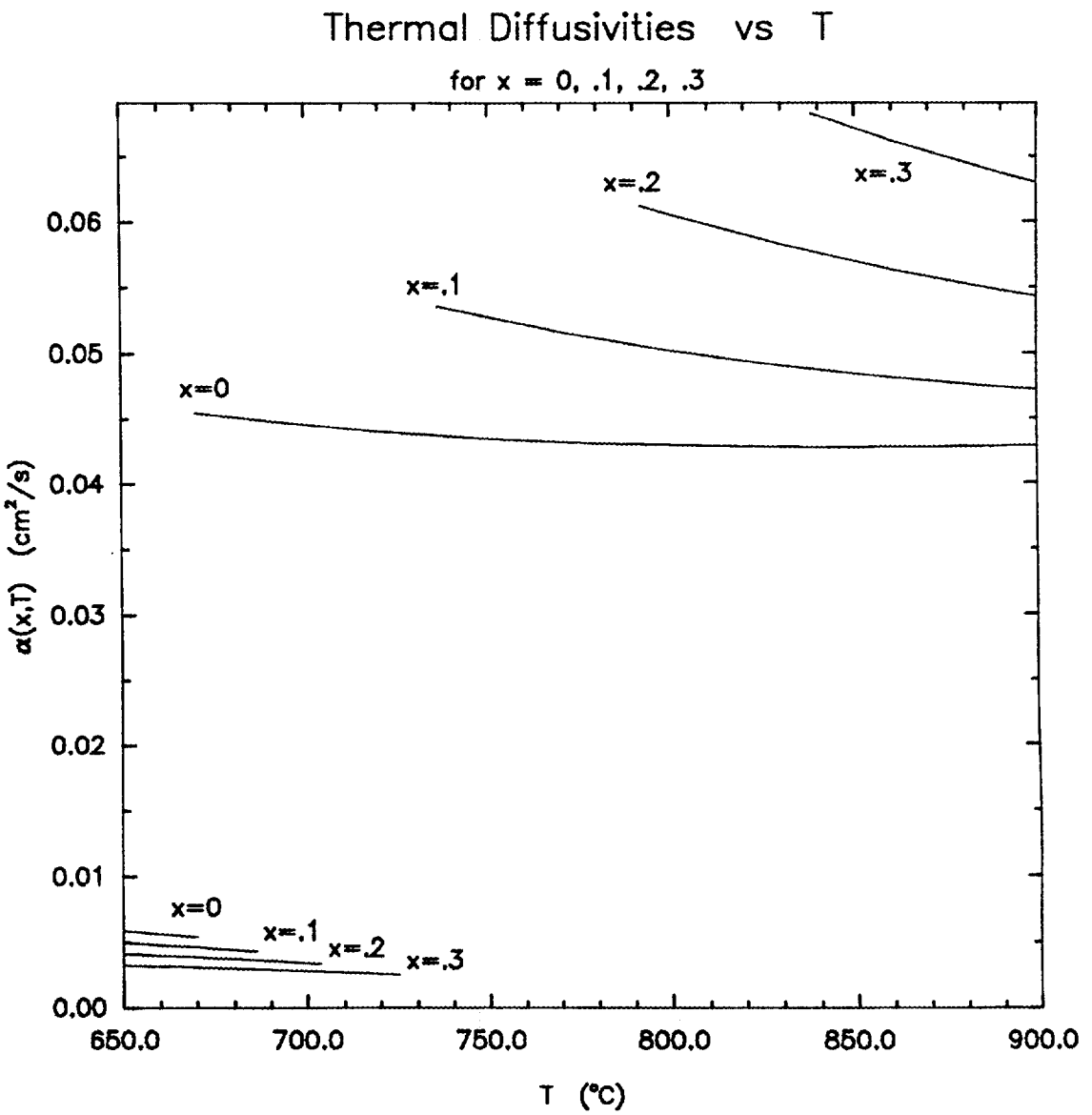
Thermal Diffusivities vs T
for x = 0, .1, .2, .3
x=.3
x=.2
x=.1
x=0
x=0
x=.1
x=.2
x=.3
0.06
0.05
0.04
0.03
0.02
0.01
0.00
α(x,T) (cm²/s)
650.0
700.0
750.0
800.0
850.0
900.0
T (°C)

Figure 6.1

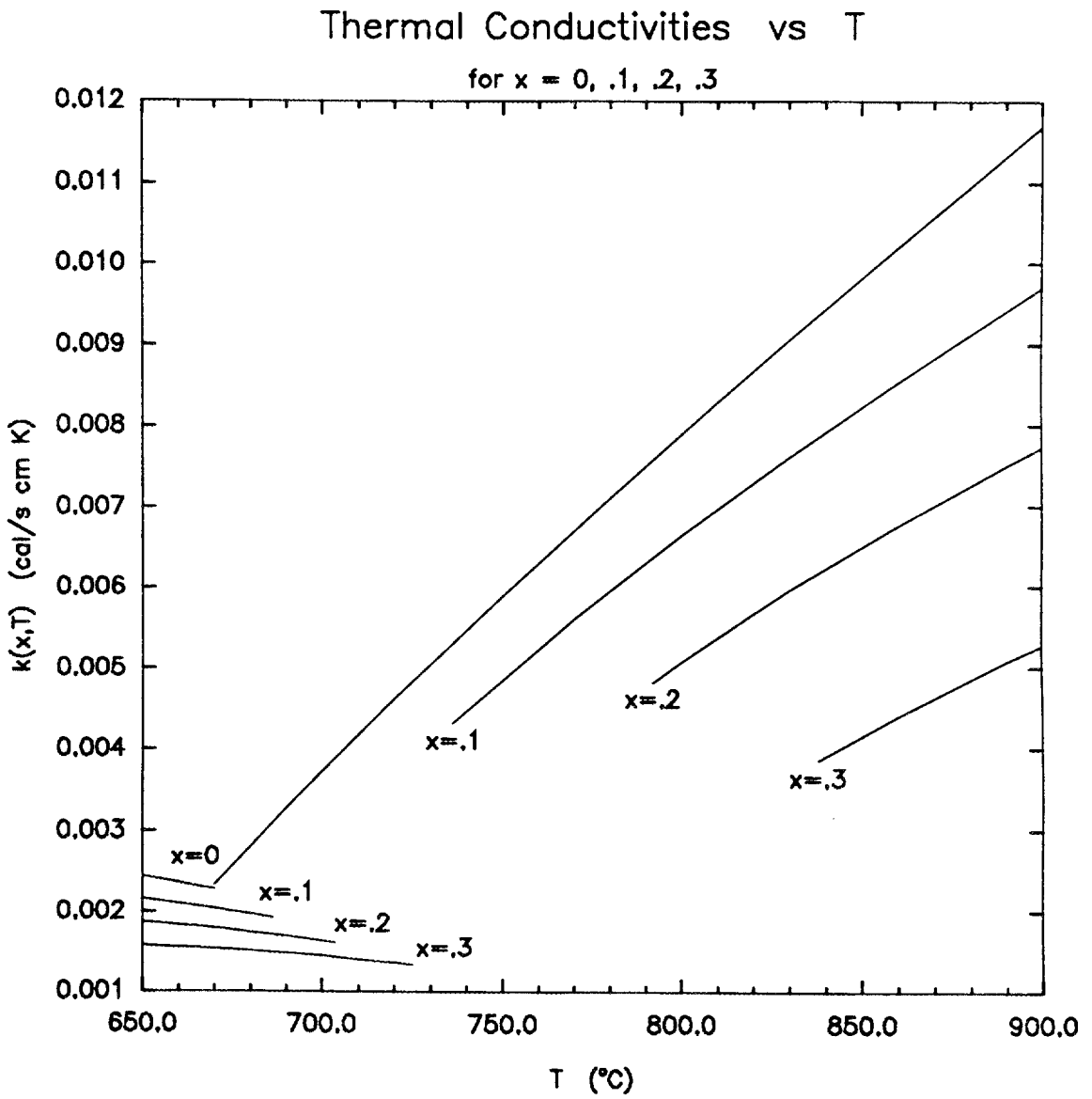
Thermal Conductivities vs T
for x = 0, .1, .2, .3
0.012
0.011
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
k(x,T) (cal/s cm K)
650.0
700.0
750.0
800.0
850.0
900.0
T (°C)
x=0
x=.1
x=.2
x=.3
x=.1
x=.2
x=.3

Figure 6.2

$$D^S(x,T) = 315 \cdot 10^{-3.53x} \exp(-\frac{22400}{T}) \quad (cm^2/s), \quad T \text{ in Kelvin} . \tag{7.2}$$

At $x = .2$, $T = 600°C$, this is of the order $5 \cdot 10^{-10}$ cm^2/s. Extrapolating the validity of (7.2) to $T = 700°C$, we find $D^S(x = .2, T = 700°C) \approx 6 \times 10^{-9}$ cm^2/s.

REFERENCES

[1] Alexiades, V., "Casting of *HgCdTe*, Part II: Conduction-Diffusion Model and its numerical implementation", Oak Ridge National Laboratory Report ORNL/TM-11753, to appear in March 1991.

[2] Brebrick, R. F., C.-H. Su and P.-K. Liao, "Associated Solution Model for *Go–In–56* and *Hg–Cd–Te*", pp. 171-253, in *Semiconductors and Semimetals*, eds. R. K. Willardson and A. C. Beer, Academic Press, New York, 1983.

[3] Chandra, D. and Holland, L. R., "Density of liquid $Hg_{1-x}Cd_xTe$", *J. Vac. Sci. Technol. A*, **1** (1983), 1620-1625.

[4] Holland, L. R. and Taylor, R. E., "Measured thermal diffusivity of $Hg_{1-x}Cd_xTe$ solids and melts", *J. Vac. Sci. Technol. A*, **1**(3) (1983), 1615-1619.

[5] Nelson, D. A., Higgins, W. M., and Lancaster, R. A. "Advances in *(Hg,Cd)Te* materials technology", *Proc. Soc. Photo-Optical Instrum. Eng.*, **225** (1980).

[6] Lehoczky, S. L., Szofran, F. R. and Martin, B. G., "Advanced methods for preparation and characterization of infrared detector materials", NASA Report CR-161598 (1980); Part II, NASA Report CR-161949 (1981).

[7] Mills, K. C., *Thermodynamics Data for Inorganic Sulptides, Selenides, and Tellurides*, Butterworths, London, 1974.

[8] Schwartz, J. P., Tung, T. and Brebrick, R. F., "Partial pressures over *HgTe–CdTe* solid solutions", *J. Electrochem. Soc.* **128** (1981), 438-451.

[9] Su, C.-H., Liao, P.-K. and Brebrick, R. F., "Partial pressures over the pseudobinary solid solution $Hg_{1-x}Cd_xTe$ for $x = 0.70$ and 0.95 and over four Te-rich ternary melts", *J. Electrochem. Soc.* **132** (4) (1985), 942-949.

[10] Su, C.-H., "Heat capacity, enthalpy of mixing, and thermal conductivity of $Hg_{1-x}Cd_xTe$ pseudobineary melts", *J. Crystal Growth*, **78** (1986), 51-77.

[11] Szofran, F. R. and Lehoczky, S. L., "The pseudobinary *HgTe–CdTe* phase diagram", *J. Electron. Mater.* **10** (1981), 1131-1149.

[12] Tung, T., Su, C.-H., Liao, P.-K. and Brebrick, R. F., "Measurement and analysis of the phase diagram and thermodynamic properties in the *HgCdTe* system", *J. Vacuum Sci. Technol.* **21** (1982), 117-124.

[13] Zanio K., and Massopust, T., "Interdiffusion in *HgCdTe/CdTe* structures", *J. Electron. Mater.* **15** (1986), 103-109.

INTERNAL DISTRIBUTION

1-5. V. Alexiades
6. B. R. Appleton
7-8. T. S. Darland/ Mathematical Sciences Library
9. M. Olszewski
10-14. S. A. Raby
15. J. J. Tomlinson
16-20. R. C. Ward
21. R. P. Wichner
22. Central Research Library
23. K-25 Library
24. ORNL Patent Office
25. Y-12 Technical Library
26. Laboratory Records - RC
27-28. Laboratory Records Department

EXTERNAL DISTRIBUTION

29. Professor Roger W. Brockett, Wang Professor of Electrical Engineering and Computer Science, Division of Applied Sciences, Harvard University, Cambridge, MA 02138
30. Dr. John Cavallini, Acting Director, Scientific Computing Staff, Applied Mathematical Sciences, Office of Energy Research, U.S. Department of Energy, Washington, DC 20585
31. Dr. Alexandre Chorin, Mathematics Department, Lawrence Berkeley Laboratory, Berkeley, CA 94720
32. Dr. James Corones, Ames Laboratory, Iowa State University, Ames, IA 50011
33. Dr. John J. Dorning (EPMD Advisory Committee), Department of Nuclear Engineering Physics, Thornton Hall, McCormick Road, University of Virginia, Charlottesville, VA 22901
34. Professor Richard E. Ewing, Department of Mathematics, University of Wyoming, Laramie, WY 82071
35. Professor James Glimm, Department of Mathematics, State University of New York, Stony Brook, NY 11794
36. Dr. Hans Kaper, Mathematics and Computer Science Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439
37. Professor Peter D. Lax, Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, NY 10012
38. Dr. Alex Lehoczky, ES 72, Space Science Laboratory, Marshall Space Flight Center, NASA, Huntsville, AL 35812

39. Dr. James E. Leiss, (EPMD Advisory Committee), 13013 Chestnut Oak Drive, Gaithersburg, MD 20878

40. Professor Neville Moray (EPMD Advisory Committee), Department of Mechanical and Industrial Engineering, University of Illinois, 1206 West Green Street, Urbana, IL 61801

41. Lee Riedinger, Director, The Science Alliance Program, University of Tennessee, Knoxville, TN 37996

42. Dr. Alan Solomon, 90 Eshel St., P.O. Box 227, Omer 84965, Israel

43. Dr. Chin-Hua Su, ES 72, Space Science Laboratory, Marshall Space Flight Center, NASA, Huntsville, AL 35812

44. Dr. Frank Szofran, ES 72, Space Science Laboratory, Marshall Space Flight Center, NASA, Huntsville, AL 35812

45. Professor Mary F. Wheeler (EPMD Advisory Committee), Department of Mathematical Sciences, Rice University, P.O. Box 1892, Houston, TX 77251

46. Office of Assistant Manager for Energy Research and Development, U.S. Department of Energy, Oak Ridge Operations Office, P.O. Box 2001, Oak Ridge, TN 37831-8600

47-56. Office of Scientific and Technical Information, P. O. Box 62, Oak Ridge, TN 37830