ADVANCED METHODS FOR PREPARATION AND CHARACTERIZATION OF INFRARED DETECTOR MATERIALS, PART I

B. S. L. Lehoczky, F. R. Szofran, and B. G. Martin
McDonnell Douglas Research Laboratories
McDonnell Douglas Corporation

Interim Report

July 5, 1980

Prepared for
NASA - Marshall Space Flight Center
Marshall Space Flight Center, Alabama 35812
The pseudobinary HgTe-CdTe phase diagram was determined by precision
differential-thermal-analysis measurements and was theoretically analyzed
in terms of a regular associated solution model. $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$ alloy
crystals were grown by a Bridgman-Stockbarger method at furnace translation
rates of 0.0685 to 5.62 $\mu$m/s. A theoretical analysis of the measured axial
compositional profiles was used to establish the liquid HgTe-CdTe inter-
diffusion coefficient and the liquid/solid-interface-temperature-gradient
to growth-rate ratio required to prevent constitutional supercooling.
Theoretical models based upon a microscopic theory of electrical conduction
and computer programs specific to $\text{Hg}_1-x\text{Cd}_x\text{Te}$ were developed for calculations
of charge-carrier concentrations, Hall coefficients, Fermi energy, and
conduction-electron mobility as functions of $x$, temperature, and ionized-
defect and neutral-defect concentrations. The measured and calculated
results were in good agreement.
This report describes the work performed from December 5, 1978, through July 5, 1980, by the McDonnell Douglas Research Laboratories (MDRL) under the National Aeronautics and Space Administration (NASA) Contract NAS8-33107. The ultimate objectives of the study are to quantitatively establish the characteristics of Hg$_{1-x}$Cd$_x$Te as grown on Earth as a basis for subsequent evaluation of the material processed in space and to develop the experimental and theoretical analytical methods required for such evaluation. The technical report was submitted to NASA in July 1980.

The work was performed in the Solid State Sciences Department, managed by Dr. C. R. Whitsett. The Principal Investigator was Dr. S. L. Lehoczky; Co-Investigators were Dr. F. R. Szofran and Dr. B. G. Martin.
## CONTENTS

1. INTRODUCTION
   1.1 Scope of Study
   1.2 Summary of Progress

2. PSEUDOBINARY HgTe-CdTe PHASE DIAGRAM
   2.1 Alloy Preparation
   2.2 Experimental Method for Differential Thermal Analyses
   2.3 Differential Thermal Analysis Results
   2.4 Error Analysis and Comparison with Previous Results
   2.5 Liquid-Solid Equilibrium Parameters

3. PHASE EQUILIBRIA CALCULATIONS
   3.1 Theoretical Model
   3.2 Regular Associated Solution Parameters for the HgCdTe Alloy System
   3.3 Component Partial Pressures over the Pseudobinary Melt

4. HIGH-TEMPERATURE-GRADIENT DIRECTIONAL SOLIDIFICATION
   4.1 Alloy Preparation
   4.2 Experimental Arrangement and Procedures for Unidirectional Crystal Growth
   4.3 Bridgman Crystal Growth Runs
   4.4 Ingot Characterization
      4.4.1 Determination of Alloy Composition by Mass Density Measurements
   4.5 Alloy Compositional Variation Along the Growth Axis
      4.5.1 Theoretical Modeling
      4.5.2 Comparison of Measured and Calculated Results

PRECEDING PAGE BLANK NOT FILMED
CONTENTS (continued)

5. THEORETICAL MODELING OF CHARGE-CARRIER CONCENTRATIONS AND ELECTRON MOBILITIES.................................65
   5.1 Energy-Band Structure and Band Parameters.................................65
   5.2 Calculation of the Temperature Dependence of the Carrier Concentrations.................................67
   5.3 Theoretical Modeling of the Electron Mobility.................................72
   5.4 Calculations of the Temperature Dependence of the Electron Mobility.................................74

REFERENCES.................................................................................................77

APPENDIX A: ELECTRON SCATTERING AND THE SOLUTION TO THE BOLTZMANN EQUATION........................................80
   A.1 Longitudinal-Optical (LO) Phonon Scattering Mechanism........................................80
   A.2 Acoustical-Phonon (ac) Scattering Mechanism........................................84
   A.3 Ionized Impurity (ii) Scattering Mechanism........................................86
   A.4 Electron-Hole (eh) Scattering Mechanism........................................88
   A.5 Compositional-Disorder (dis.) Scattering Mechanism........................................88
   A.6 Neutral-Defect (nd) Scattering Mechanism........................................89
   A.7 Calculation of Electron Mobility........................................89

APPENDIX B: COMPUTER PROGRAM FOR CALCULATION OF CHARGE-CARRIER CONCENTRATIONS AND ELECTRON MOBILITIES.................................93
   B.1 Description of Symbols - Main Program........................................93
   B.2 Description of Symbols - Subroutine Programs........................................96
   B.3 Computer Program Flow Charts........................................100
   B.4 Computer Program........................................141
**LIST OF ILLUSTRATIONS**

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Experimental arrangement for differential thermal analysis measurements</td>
<td>7</td>
</tr>
<tr>
<td>2. Electronic instrumentation for differential thermal analysis</td>
<td>7</td>
</tr>
<tr>
<td>3. Rate dependence of thermal arrest for HgTe</td>
<td>9</td>
</tr>
<tr>
<td>4. Differential thermal analysis data for Hg$<em>{0.9}$Cd$</em>{0.1}$Te</td>
<td>10</td>
</tr>
<tr>
<td>5. Differential thermal analysis data for Hg$<em>{0.8}$Cd$</em>{0.2}$Te</td>
<td>11</td>
</tr>
<tr>
<td>6. DTA data for $x = 0.1, 0.2, 0.3$, $0.4, 0.6, 0.7, 0.8,$ and $0.9$ Hg$_{1-x}$Cd$_x$Te alloys</td>
<td>12</td>
</tr>
<tr>
<td>7. Hg$_{1-x}$Cd$_x$Te melting curves as observed</td>
<td>13</td>
</tr>
<tr>
<td>8. Hg$_{1-x}$Cd$_x$Te phase diagram</td>
<td>17</td>
</tr>
<tr>
<td>9. Comparison of present phase-equilibria data with previous results</td>
<td>20</td>
</tr>
<tr>
<td>10. Temperature dependence of the interface distribution coefficient</td>
<td>21</td>
</tr>
<tr>
<td>11. Composition dependence of the distribution coefficient</td>
<td>22</td>
</tr>
<tr>
<td>12. Temperature dependence of the alloy liquid fraction for various alloy compositions</td>
<td>23</td>
</tr>
<tr>
<td>13. The temperature dependence of the rate of change with respect to temperature of the alloy liquid fraction for various alloy compositions</td>
<td>24</td>
</tr>
<tr>
<td>14. Compositional variation of the observed DTA signals as a function of sample temperature</td>
<td>24</td>
</tr>
<tr>
<td>15. Component partial pressures over the Hg$_{1-x}$Cd$_x$Te melt</td>
<td>34</td>
</tr>
<tr>
<td>16. The temperature variation of Hg partial pressure over the Hg$_{1-x}$Cd$_x$Te melt as a function of Cd fraction</td>
<td>35</td>
</tr>
<tr>
<td>17. Bridgman crystal-growth furnace assembly</td>
<td>37</td>
</tr>
<tr>
<td>18. Temperature profile of crystal-growth furnace during growth of ingot L3</td>
<td>39</td>
</tr>
<tr>
<td>19. Temperature profile of crystal-growth furnace during growth of ingot L4</td>
<td>40</td>
</tr>
</tbody>
</table>
LIST OF ILLUSTRATIONS (continued)

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>20. Temperature profile of crystal-growth furnace during growth of ingots L6 and L7</td>
<td>40</td>
</tr>
<tr>
<td>21. (a) Location of wafers along the growth axis of ingot L6 and (b) the IR measurement positions for a wafer</td>
<td>47</td>
</tr>
<tr>
<td>22. Typical transmission spectra for a wafer (A26) from ingot L6</td>
<td>48</td>
</tr>
<tr>
<td>23. Radial variations of the cut-on wavelength and Cd composition for ingot L6</td>
<td>48</td>
</tr>
<tr>
<td>24. Radial variation of wavelength at 50% relative transmission across slices from ingot L6</td>
<td>49</td>
</tr>
<tr>
<td>25. The variation of the interface segregation coefficient and interface translation rate along the growth axis of ingot L3</td>
<td>53</td>
</tr>
<tr>
<td>26. The variation of the interface segregation coefficient and interface translation rate along the growth axis of ingot L4</td>
<td>54</td>
</tr>
<tr>
<td>27. The variation of the interface segregation coefficient and interface translation rate along the growth axis of ingot L6</td>
<td>55</td>
</tr>
<tr>
<td>28. A comparison between the measured and calculated compositional profiles for ingot L3</td>
<td>56</td>
</tr>
<tr>
<td>29. A comparison between the measured and calculated compositional profiles for ingot L4</td>
<td>57</td>
</tr>
<tr>
<td>30. A comparison between the measured and calculated compositional profiles for ingot L6</td>
<td>58</td>
</tr>
<tr>
<td>31. A comparison between the experimental data for ingot L3 and calculated results for various values of the diffusion coefficient</td>
<td>59</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>32.</td>
<td>A comparison between the experimental data for ingot L4 and calculated results for various values of the diffusion coefficient.</td>
</tr>
<tr>
<td>33.</td>
<td>A comparison between the experimental data for ingot L6 and calculated results for various values of the diffusion coefficient.</td>
</tr>
<tr>
<td>34.</td>
<td>A comparison between the experimental data for ingot L3 and calculated results for a diffusion coefficient of $6.0 \times 10^{-5}$ cm$^2$/s and constant $k$, $R$.</td>
</tr>
<tr>
<td>35.</td>
<td>A comparison between the experimental data for ingot L4 and the calculated results for a diffusion coefficient of $6.0 \times 10^{-5}$ cm$^2$/s and constant $k$, $R$.</td>
</tr>
<tr>
<td>36.</td>
<td>A comparison between the experimental data for ingot L6 and the calculated results for a diffusion coefficient of $4.5 \times 10^{-5}$ cm$^2$/s and constant $k$, $R$.</td>
</tr>
<tr>
<td>37.</td>
<td>Theoretical and experimental conduction-electron concentration for Hg$<em>{0.817}$Cd$</em>{0.183}$Te.</td>
</tr>
<tr>
<td>38.</td>
<td>A comparison of the temperature dependence of the calculated and measured conduction-electron mobilities for an alloy composition of $x = 0.183$.</td>
</tr>
<tr>
<td>39.</td>
<td>A comparison of the temperature dependence of the calculated and measured conduction-electron mobilities for an alloy composition of $x = 0.183$.</td>
</tr>
</tbody>
</table>
# LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Alloy samples prepared for the phase-diagram determinations</td>
<td>5</td>
</tr>
<tr>
<td>2. Elemental constituents of alloys used for the phase diagram determination</td>
<td>6</td>
</tr>
<tr>
<td>3. Measured phase-equilibria data for Hg$_{1-x}$Cd$_x$Te</td>
<td>15</td>
</tr>
<tr>
<td>4. Free-volume correction parameters and corrected liquidus temperatures</td>
<td>16</td>
</tr>
<tr>
<td>5. Liquidus and solidus temperatures for Hg$_{1-x}$Cd$_x$Te</td>
<td>17</td>
</tr>
<tr>
<td>6. Uncertainties of the solidus and liquidus temperatures</td>
<td>18</td>
</tr>
<tr>
<td>7. Best values for the fitting constants C$_1$ and D$_1$</td>
<td>21</td>
</tr>
<tr>
<td>8. R.A.S. parameters and thermodynamic data for the Hg-Cd-Te system</td>
<td>30</td>
</tr>
<tr>
<td>9. A comparison of experimental and calculated temperatures for Hg$_{1-x}$Cd$_x$Te</td>
<td>31</td>
</tr>
<tr>
<td>10. Mole fractions of species in liquid phase as functions of temperature</td>
<td>31</td>
</tr>
<tr>
<td>11. Calculated component partial pressures over the Hg$_{1-x}$Cd$_x$Te melt</td>
<td>33</td>
</tr>
<tr>
<td>12. Average alloy compositions for various positions along the axis of ingot L3</td>
<td>44</td>
</tr>
<tr>
<td>13. Average alloy compositions for various positions along the axis of ingot L4</td>
<td>45</td>
</tr>
<tr>
<td>14. Average alloy compositions for various positions along the axis of ingot L6</td>
<td>46</td>
</tr>
<tr>
<td>15. Parameters for electron-mobility and charge-carrier-concentration calculation for Hg$_{1-x}$Cd$_x$Te alloys</td>
<td>70</td>
</tr>
</tbody>
</table>
1. INTRODUCTION

1.1 Scope of Study

The overall study includes the entire range, \(0 < x < 1\), of \(\text{Hg}_{1-x}\text{Cd}_x\text{Te}\) alloy compositions. Crystals were prepared by the Bridgman method with a wide range of crystal growth rates and temperature gradients adequate to prevent constitutional supercooling under diffusion-limited, steady-state, growth conditions. The longitudinal compositional gradients for different growth conditions and alloy compositions were calculated and compared with experimental data to develop a quantitative model of the crystal growth kinetics for the \(\text{Hg}_{1-x}\text{Cd}_x\text{Te}\) alloys, and measurements were performed to ascertain the effect of growth conditions on radial compositional gradients. The pseudobinary \(\text{HgTe-CdTe}\) constitutional phase diagram was determined by precision differential-thermal-analysis measurements and used to calculate the segregation coefficient of \(\text{Cd}\) as a function of \(x\) and interface temperature. Experiments will be conducted and theoretical analysis will be performed during the next phase of the program to determine the ternary phase equilibria in selected regions of the \(\text{Hg-Cd-Te}\) constitutional phase diagram, and electron and hole mobilities as functions of temperature will be analyzed to establish charge-carrier scattering probabilities. Computer algorithms specific to \(\text{Hg}_{1-x}\text{Cd}_x\text{Te}\) were developed for calculations of the charge-carrier concentrations, charge-carrier mobilities, Hall coefficient, optical absorptance, and Fermi energy as functions of \(x\), temperature, ionized donor and acceptor concentrations, and neutral-defect concentrations.

1.2 Summary of Progress

A series of differential-thermal-analysis (DTA) measurements was performed for \(\text{Hg}_{1-x}\text{Cd}_x\text{Te}\) alloy compositions with \(x = 0, 0.1, 0.2, 0.3, 0.4, 0.6, 0.7, 0.8, 0.9,\) and 1.0. The liquidus and solidus temperatures deduced from the DTA data were used to establish the pseudobinary \(\text{HgTe-CdTe}\) constitutional phase diagram. The segregation coefficient of \(\text{Cd}\) was determined as a function of \(x\) and interface temperature.

Iterative phase-equilibria calculations based on the regular associated solution (R.A.S.) theory\(^1,^2\) were performed, and a set of R.A.S. parameters was
obtained by simultaneously least-squares-fitting the binary Hg-Te and Cd-Te \textsuperscript{3-6} and pseudobinary HgTe-CdTe phase diagrams. The R.A.S. parameters were used to calculate the activities of Hg, Cd, and Te\textsubscript{2} and their partial pressures over pseudobinary melts. The calculated mercury partial pressures are in reasonable agreement with Steininger's experimental results.\textsuperscript{7} The validity of the R.A.S. parameters and thus the calculated partial pressures are sensitively dependent upon necessary assumptions in the calculations; for example, negligible Te-Te association in the melt was assumed.

Hg\textsubscript{0.8}Cd\textsubscript{0.2}Te alloy crystals were grown by the Bridgman method at constant furnace translation rates of 0.0685, 0.310, 0.597, 1.12, and 5.62 \textmu m/s. The temperature gradients at the solid-liquid interface, except for the 5.62 \textmu m/s growth rate, were adequate to prevent constitutional supercooling in the melts. For three of the ingots, the longitudinal compositional profiles were determined by precision density measurements and were compared with calculated profiles\textsuperscript{8} for various assumed values of D, the liquid HgTe-CdTe interdiffusion coefficient. The calculations included the variations in the interface translation rates and interface segregation coefficients during the growth process. These variations were calculated from the temperature profiles measured prior to each growth run, the measured compositional profiles, and phase equilibria data. The best fits to the data for the alloys with x = 0.2 yielded 5.5 x 10\textsuperscript{-5} cm\textsuperscript{2}/s for D and 1.5 x 10\textsuperscript{6} K/s/cm\textsuperscript{2} for G/R, the interface-temperature-gradient to growth-rate ratio required to prevent constitutional supercooling. Radial compositional variations were measured on thin slices from several ingots by infrared (IR) transmission-edge mapping. The radial compositional profiles deduced from the cut-on wavelengths implied concave solid/liquid interfaces for the entire lengths of the crystals.

Theoretical models and computer programs specific to Hg\textsubscript{1-x}Cd\textsubscript{x}Te were developed for calculations of charge-carrier concentrations, Hall coefficient, Fermi energy, and conduction-electron mobility as functions of \textit{x}, temperature, and ionized-defect and neutral-defect concentrations. As in previous work on the HgCdSe alloy system\textsuperscript{9,10} the Kane three-band model\textsuperscript{11} was used to describe the band structure of the HgCdTe alloys, and the best available band parameters were compiled from the literature. The temperature dependence of the electron concentration was calculated for various net donor concentrations from 4.2 K to 300 K, and the calculated results agreed well with available data.
The mobility calculations included the following intrinsic scattering mechanisms: longitudinal-optical phonon, longitudinal and transverse-acoustical phonon, heavy-hole, and alloy disorder potential. The extrinsic scattering mechanisms included charged and neutral point-defects. A comparison of calculated results with available experimental data indicated that longitudinal optical-phonon and charged and neutral defect scattering are the dominant mobility-limiting mechanisms.
2. PSEUDOBINARY HgTe-CdTe PHASE DIAGRAM

2.1 Alloy Preparation

The HgTe-CdTe alloys used for the phase diagram determinations were prepared by reacting the constituent elements in sealed, fused-silica, 5-mm i.d. x 10-mm o.d. ampules. The ampules were cleaned and etched in aqueous HF and annealed at 1150°C in vacuum to remove residual contaminants. Square cross-section bars of 99.9999% pure Cd and Te were cut from large ingots. The Cd bars were etched in concentrated HNO₃ and repeatedly rinsed in methanol. The Te bars were etched in Br₂ and repeatedly rinsed in methanol. The ampules were loaded in a vertical position first with 99.9999% pure Hg, then Te, and finally Cd. This procedure prevented contact between Hg and Cd in the presence of air. The ampules were evacuated and backfilled with He several times before final evacuation and sealing. Using the above procedure, little or no wetting occurred between the ampule and the alloy during reaction of the elements. In many cases, the reacted alloy would slide inside the ampule.

The various alloy preparations used for the phase diagram determinations are summarized in Table 1. As implied by the table, a substantial number of prepared ampules were discarded for various reasons. Following a series of initial experimental runs, a concentrated effort was undertaken to increase the fill factor (reduce the free-volume) of the ampules. For this purpose, a series of alloys was cast, the ampules were reopened, solid quartz rods were placed in the ampules, and the ampules were resealed. For the ampules containing alloy compositions of $x = 0.1$ and 0.2, the rod diameters were 4 mm. For alloy compositions with $x$-values of 0.3 to 0.9, 5-mm diameter rods, etched in concentrated hydrofluoric acid to achieve close fits, were used. With the exceptions of the 0.1 and 0.2 alloys, this sealing procedure repeatedly resulted in ampule ruptures at the measurement temperatures, and the cause of these failures is unclear.

In subsequent preparations of alloys in the high-$x$ range, an increase of the alloy volume in the ampule was used to increase the ampule fill-factor. The alloy constituents for the ampules that served as samples for the majority of the measurements described in this report are listed in Table 2.
### TABLE 1. ALLOY SAMPLES PREPARED FOR THE PHASE-DIAGRAM DETERMINATIONS.

<table>
<thead>
<tr>
<th>Sample no.</th>
<th>Composition (x)</th>
<th>Quantity (moles)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>0.02</td>
<td>A, B</td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>0.02</td>
<td>A, B</td>
</tr>
<tr>
<td>3</td>
<td>0.2</td>
<td>0.06</td>
<td>A, C</td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>0.06</td>
<td>A, C</td>
</tr>
<tr>
<td>5</td>
<td>0.4</td>
<td>0.06</td>
<td>A, B, C</td>
</tr>
<tr>
<td>6</td>
<td>0.3</td>
<td>0.06</td>
<td>A, C</td>
</tr>
<tr>
<td>7</td>
<td>0.5</td>
<td>0.06</td>
<td>A</td>
</tr>
<tr>
<td>8</td>
<td>0.6</td>
<td>0.06</td>
<td>A</td>
</tr>
<tr>
<td>9</td>
<td>0.7</td>
<td>0.06</td>
<td>A, B</td>
</tr>
<tr>
<td>10</td>
<td>0.8</td>
<td>0.06</td>
<td>A, B</td>
</tr>
<tr>
<td>11</td>
<td>0.9</td>
<td>0.06</td>
<td>B</td>
</tr>
<tr>
<td>12</td>
<td>0.8</td>
<td>0.06</td>
<td>B</td>
</tr>
<tr>
<td>13</td>
<td>0.2</td>
<td>0.06</td>
<td>C</td>
</tr>
<tr>
<td>14</td>
<td>0</td>
<td>0.06</td>
<td>A, C</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>0.06</td>
<td>D</td>
</tr>
<tr>
<td>16</td>
<td>1.0</td>
<td>0.03</td>
<td>D</td>
</tr>
<tr>
<td>17</td>
<td>0.7</td>
<td>0.06</td>
<td>B</td>
</tr>
<tr>
<td>18</td>
<td>0.5</td>
<td>0.06</td>
<td>C, F</td>
</tr>
<tr>
<td>19</td>
<td>0.7</td>
<td>0.06</td>
<td>C, F</td>
</tr>
<tr>
<td>20</td>
<td>0.8</td>
<td>0.06</td>
<td>C, F</td>
</tr>
<tr>
<td>21</td>
<td>0.1</td>
<td>0.06</td>
<td>D</td>
</tr>
<tr>
<td>22</td>
<td>0.2</td>
<td>0.06</td>
<td>D</td>
</tr>
<tr>
<td>23</td>
<td>0.3</td>
<td>0.06</td>
<td>C, F</td>
</tr>
<tr>
<td>24</td>
<td>0.4</td>
<td>0.06</td>
<td>D</td>
</tr>
<tr>
<td>25</td>
<td>0.9</td>
<td>0.06</td>
<td>C, F</td>
</tr>
<tr>
<td>26</td>
<td>0.8</td>
<td>0.06</td>
<td>C</td>
</tr>
<tr>
<td>27</td>
<td>0.9</td>
<td>0.06</td>
<td>C</td>
</tr>
<tr>
<td>28</td>
<td>0.9</td>
<td>0.12</td>
<td>D</td>
</tr>
<tr>
<td>29</td>
<td>0.8</td>
<td>0.12</td>
<td>D</td>
</tr>
<tr>
<td>30</td>
<td>0.7</td>
<td>0.12</td>
<td>C</td>
</tr>
<tr>
<td>31</td>
<td>0.6</td>
<td>0.12</td>
<td>C</td>
</tr>
<tr>
<td>32</td>
<td>0.6</td>
<td>0.12</td>
<td>C</td>
</tr>
<tr>
<td>33</td>
<td>0.7</td>
<td>0.12</td>
<td>C</td>
</tr>
<tr>
<td>34</td>
<td>0.5</td>
<td>0.12</td>
<td>C</td>
</tr>
<tr>
<td>35</td>
<td>0.3</td>
<td>0.06</td>
<td>D</td>
</tr>
<tr>
<td>36</td>
<td>0.5</td>
<td>0.06</td>
<td>C</td>
</tr>
<tr>
<td>37</td>
<td>0.6</td>
<td>0.06</td>
<td>C</td>
</tr>
<tr>
<td>38</td>
<td>0.5</td>
<td>0.06</td>
<td>C</td>
</tr>
<tr>
<td>39</td>
<td>0.6</td>
<td>0.06</td>
<td>D</td>
</tr>
<tr>
<td>40</td>
<td>0.7</td>
<td>0.06</td>
<td>D</td>
</tr>
</tbody>
</table>

- **A**: Used for preliminary experiments
- **B**: Some sticking of alloy to ampule
- **C**: Ampule burst
- **D**: Used for measurements reported here
- **E**: 0.4 mm diam rod sealed inside after reacting alloy
- **F**: As E, except that an HF-etched 0.5-mm rod was used
TABLE 2. ELEMENTAL CONSTITUENTS OF ALLOYS USED FOR THE PHASE DIAGRAM DETERMINATION. MASS MEASUREMENT ACCURACY IS ±0.56 mg.

<table>
<thead>
<tr>
<th>Composition (%)</th>
<th>Hg (g)</th>
<th>Cd (g)</th>
<th>Te (g)</th>
<th>Stoichiometric Hg (g)</th>
<th>Excess Hg (mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>10.8349</td>
<td>0.6732</td>
<td>7.6555</td>
<td>10.8345</td>
<td>0.4</td>
</tr>
<tr>
<td>0.2</td>
<td>9.6299</td>
<td>1.3501</td>
<td>7.6570</td>
<td>9.6289</td>
<td>1.0</td>
</tr>
<tr>
<td>0.3</td>
<td>9.5487</td>
<td>2.2950</td>
<td>8.6748</td>
<td>9.5428</td>
<td>5.9</td>
</tr>
<tr>
<td>0.4</td>
<td>7.2201</td>
<td>2.6992</td>
<td>7.6555</td>
<td>7.2190</td>
<td>1.1</td>
</tr>
<tr>
<td>0.6</td>
<td>4.5719</td>
<td>3.8343</td>
<td>7.2582</td>
<td>4.5687</td>
<td>3.2</td>
</tr>
<tr>
<td>0.7</td>
<td>3.6452</td>
<td>4.7582</td>
<td>7.7183</td>
<td>3.6433</td>
<td>1.9</td>
</tr>
<tr>
<td>0.8</td>
<td>4.7977</td>
<td>10.7427</td>
<td>15.2430</td>
<td>4.7939</td>
<td>3.8</td>
</tr>
<tr>
<td>0.9</td>
<td>2.4053</td>
<td>12.1474</td>
<td>15.3200</td>
<td>2.4083</td>
<td>1.0</td>
</tr>
</tbody>
</table>

2.2 Experimental Method for Differential Thermal Analyses

Differential thermal analysis (DTA) measurements were used for the determination of the phase equilibria temperatures. The experimental arrangement of the ampules in the DTA furnace is shown in Figure 1.

An ampule containing the alloy sample is mounted end-to-end with a second ampule coaxially inside the 460-mm long isothermal furnace liner (Na heat pipe) and the 610-mm long tube furnace. The second ampule contains antimony, which in addition to serving as the reference heat capacity provides a thermocouple calibration point for each experimental run. The ampules are held on axis by a quartz centering fixture (not shown in the figure). The annular volume between the ampules and a 25-mm o.d. quartz tube is filled with powdered diatomaceous earth. The 25-mm tube is inside an Inconel tube, which prevents damage to the heat pipe and furnace in case of ampule failure.

Both the alloy and Sb-reference ampules are fitted with a Pt-foil band ~5-mm wide and positioned near the middle of the ampule axially. The two junctions of a type-K differential thermocouple are secured to the bands. A separate type-K thermocouple is secured to the band on the Sb-reference ampule. Each thermocouple lead extends to a copper junction maintained in a triple-point-of-water cell. A block diagram of the furnace control and data acquisition instrumentation is shown in Figure 2. The temperature of the Sb-reference sample was monitored on the x-axis, and the differential
Figure 1. Experimental arrangement for differential thermal analysis measurements.

thermocouple output on the y-axis of an x-y recorder. Each graph-paper used for data recording was calibrated by drawing vertical lines at 1-mV intervals by driving the x-axis with a potentiometer (Leeds and Northrop model 8691). This potentiometer was in turn periodically checked against another potentiometer (Leeds and Northrop K-4) and verified to be accurate to within ±20 μV. The output of a type-K thermocouple is approximately 40 μV/deg.

Figure 2. Electronic instrumentation for differential thermal analysis.
The temperature programmer allows the furnace temperature to be changed at a uniform rate and turns the x-y recorder servo and pen-lift on and off. The furnace protection circuit, a meter relay which drives a power relay, provides an additional margin of safety against excessive furnace temperatures.

A thermocouple calibration facility, similar to that described in NBS Circular 59012, using graphite crucibles and NBS reference materials was constructed and used to calibrate thermocouple wire lots used for the measurements. The melting-temperature reference materials were Zn, Al, and Cu. The melting temperature of t'-Sb-reference sample served as an internal calibration temperature, and the Sb melting point was checked at least once prior to each experimental run.

2.3 Differential Thermal Analysis Results

Generally, for DTA measurements, the output signal from the differential sensors varies directly with the heating/cooling rates used, i.e., high heating/cooling rates yield larger signals and thus better signal to noise ratios. Measurements made at too high heating/cooling rates, however, can significantly alter the details of the DTA curves, thereby yielding phase transformation temperatures that do not reflect true equilibrium values. To assure that heating/cooling rates used in this study were within the allowable range, HgTe calibration sample test runs were made at a series of heating rates (0.5, 1, 2, 3, 4, and 5°C/min). The thermal arrest curves for the various runs are shown in Figure 3. The melting temperatures deduced from the heating curves are within ±1.7°C of 669.5°C for the different heating rates, and there is no evidence for systematic variation of the onset of thermal-arrest with heating rate. Because the maximum cooling rate of the furnace at or below 670°C was about 3°C/min, all alloy heating and cooling curves were recorded at a rate of 2°C/min in order to enhance the differential thermocouple outputs while allowing identical heating and cooling rates.

Alloy inhomogeneities broaden the range of temperatures over which transformations occur and thus introduce significant uncertainties into the phase equilibria temperatures as deduced from DTA. For this reason, the samples were always rapidly quenched following casting and uniformly cooled.
after each DTA run to reduce the possibility of preferential alloy segregation along the a-pole axis. To eliminate radial alloy inhomogeneities, the samples were annealed at temperatures, $T_A$, just below their solidus values. To ascertain the minimum annealing times required, samples with $x = 0.1, 0.2, 0.8$ and 0.9 were annealed for successively longer annealing times from 1 to 60 h, and a DTA run was made following each anneal. An increase in the annealing time from 1 to 15 h always resulted in a significant sharpening of the DTA
curves in the vicinity of the apparent solidus temperatures, which indicates that the annealing effected alloy homogenization by diffusion. On the other hand, the changes caused by increasing the annealing time beyond 30 h were usually negligible, as shown for samples with \( x = 0.1 \) and 0.2 in Figures 4 and 5, respectively, where \( T_A \) and \( T_L \) correspond respectively to the annealing and liquidus temperatures, and the symbols 1, 2, 3, and 4 designate the DTA curves that were obtained following annealing times of 1, 15, 30 and 60 h, respectively.

DTA curves for fully annealed samples with \( x = 0.1, 0.2, 0.3, 0.4, 0.6, 0.7, 0.8, \) and 0.9 are shown in Figure 6, and the collection of melting curves is shown in Figure 7. The horizontal axis shows the measured Sb-reference ampule temperature, \( T \), and the vertical axis gives differential temperatures, \( S \), for the alloy ampule as measured with respect to \( T \).

Figure 4. Differential thermal analysis data for \( H_{0.9}Cd_{0.1}Te \).
\[ \frac{dT}{dt} = 2^\circ \text{C/min} \]

Figure 5. Differential thermal analysis data for Hg$_{0.8}$Cd$_{0.2}$Te.
Figure 6. DTA data for x = 0.1, 0.2, 0.3, 0.4, 0.6, 0.7, 0.8 and 0.9 Hg$_x$Cd$_{1-x}$Te alloys.
Considering radiation heat transfer only, the heat balance at the outer wall of the sample ampule yields

\[ \varepsilon_F T_F^4 - \varepsilon_p T_1^4 = \frac{r_s}{r_q} (\varepsilon_p T_1^4 - \varepsilon_s T_s^4), \]  

where \( T_F, T_1, \) and \( T_s \) are the furnace, sample thermocouple, and sample temperatures, respectively, \( \varepsilon_F, \varepsilon_p, \) and \( \varepsilon_s \) are the furnace, sample, and quartz emissivities, respectively, and \( r_s \) and \( r_q \) are the inner and outer radii, respectively, of the quartz ampules. The measured differential thermocouple signal is given by \( S = T_1 - T. \) For steady-state conditions where the furnace temperature increases at a constant rate, \( T = T_F + P', \) where \( P' \) is a constant. Using the approximations

\[ T_1^4 = (T + S)^4 = T^4 + 4ST^3 \]  

and

\[ T_F^4 = (T + P')^4 = T^4 + 4P'T^3, \]
Equation (1) yields

$$T_s^4 = T^4 \left[ \left( 1 + \frac{r_q}{r_s} \right) \frac{\epsilon_p}{\epsilon_s} - \frac{r_q}{r_s} \frac{\epsilon_F}{\epsilon_s} \right] + 4ST^3 \left( 1 + \frac{r_q}{r_s} \right) \frac{\epsilon_p}{\epsilon_s} - 4P'T^3 \frac{r_q}{r_s} \frac{\epsilon_F}{\epsilon_s}. \tag{4}$$

A first-order expansion in $T/T$ and $P'/T$ yields

$$T_s = a_1 T + a_2 S - a_3 P', \tag{5}$$

where $a_1$, $a_2$, and $a_3$ are functions of $r_q/r_s$, $\epsilon_p/\epsilon_s$, and $\epsilon_F/\epsilon_s$.

For HgTe the observed empirical correlation between $T$, $S$, and $T_s$ is given by

$$T_s = T + 2S - P. \tag{6}$$

For CdTe also, $a_2$ was found to be 2. In the case of a nonzero baseline, $S_0$, $T_s$ is given by

$$T_s = T - S_0 + 2S - P. \tag{7}$$

$P$ is primarily the temperature drop across the ampule wall, but this term also includes thermocouple calibration corrections. In the absence of a phase transition, $T_s = T + S_0 - P$, i.e., the sample temperature is equal to the reference thermocouple temperature plus the differential temperature minus the temperature drop across the ampule wall.

For each sample, $P$ was determined by the difference between the observed and actual melting points of the Sb-reference. The values measured for $P$ using other calibration samples with known melting points ranged from 1.3°C to 3.4°C, which agree reasonably with finite-difference calculations that include both radiation and conduction heat transfer.

The solidus temperatures were determined by reploting the data of Figure 6 as a function of $T_s$ instead of $T$, using Equation (7). The solidus temperatures for $0.1 < x < 0.7$ were determined by extrapolating the initial, straight-line part of the replotted melting curves to the extended baseline. For $x = 0.8$ and 0.9, the initial departure from the baseline was used because the melting curves had no straight-line sections even when replotted as functions of $T_s$. The liquidus points, in all cases, were considered to be the temperatures at which the melting curves broke suddenly toward the baseline. The observed phase equilibrium data are listed in Table 3.
TABLE 3. MEASURED PHASE-EQUILIBRIA DATA FOR Hg$_{1-x}$Cd$_x$Te.

<table>
<thead>
<tr>
<th>Composition (x)</th>
<th>$S_0$ at solidus (°C)</th>
<th>$S_0$ at liquidus (°C)</th>
<th>P (°C)</th>
<th>Observed solidus temperature (°C)</th>
<th>Observed liquidus temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.5</td>
<td>-1.5</td>
<td>2.9</td>
<td>690</td>
<td>733</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4</td>
<td>-1.0</td>
<td>2.9</td>
<td>706</td>
<td>791</td>
</tr>
<tr>
<td>0.3</td>
<td>1.4</td>
<td>0.7</td>
<td>2.9</td>
<td>727</td>
<td>841</td>
</tr>
<tr>
<td>0.4</td>
<td>0.9</td>
<td>0.3</td>
<td>3.4</td>
<td>748</td>
<td>882</td>
</tr>
<tr>
<td>0.6</td>
<td>0.3</td>
<td>-0.3</td>
<td>1.3</td>
<td>810</td>
<td>952</td>
</tr>
<tr>
<td>0.7</td>
<td>0.7</td>
<td>-0.4</td>
<td>2.9</td>
<td>850</td>
<td>990</td>
</tr>
<tr>
<td>0.8</td>
<td>0.9</td>
<td>0.3</td>
<td>2.9</td>
<td>904</td>
<td>1022</td>
</tr>
<tr>
<td>0.9</td>
<td>3.4</td>
<td>-1.0</td>
<td>2.9</td>
<td>950</td>
<td>1051</td>
</tr>
</tbody>
</table>

Each ampul contained a small free volume. Because the partial vapor pressure of Hg over the alloy melt is much larger than the partial pressures of Cd and Te, the preferential evaporation of mercury into the ampule free volume alters both the Te/metal and Cd/Hg fractions. As suggested by the decrease in the binary Hg-Te and Cd-Te liquidus temperatures with increasing Te composition immediately above the 50 at.% Te composition, an increase in the Te/metal fraction can significantly affect the liquidus temperature. The Cd-Te liquidus temperature decreases at $\approx 10^\circ$C/at.% Te, and the Hg-Te liquidus temperature decreases at $1.2^\circ$C/at.% Te.

The following procedure was used to correct for the small Te-metal excess in the melt caused by preferential evaporation of Hg into the ampule free volume. Following the casting of an alloy, the free volume was estimated by measuring the length of the free space in the ampule. The amount of Hg in the gas phase was determined by using Steininger's empirical relationship for the Hg partial pressure, $P$, given by

$$P = P_0 \exp(21.732 - T_0/T),$$

where $P_0 = 1$ Pa and $T_0 = 7.149$ K. The number of moles of Hg, $n_{\text{Hg}}$, remaining in the melt was obtained by subtracting the amount of Hg in the vapor from the amount loaded into the ampule. The actual Te/metal mole fraction in the melt at the observed liquidus temperature is then $n_{\text{Te}}/(n_{\text{Hg}} + n_{\text{Cd}} + n_{\text{Te}})$, where $n_{\text{Cd}}$ and $n_{\text{Te}}$ are respectively the number of moles of Cd and Te in the melt. The relatively small amounts of Cd and Te$_2$ in the vapor were neglected, and the
values of \( n_{\text{Cd}} \) and \( n_{\text{Te}} \) were assumed to be the same as originally placed in the ampule. The corrections to the observed liquidus temperatures were then obtained from the expression

\[
\epsilon = \left[ \frac{n_{\text{Te}}}{n_{\text{Hg}} + n_{\text{Cd}} + n_{\text{Te}}} \right] - 0.5 \ (1.2 + 8.8x),
\]

which is based on a linear interpolation between Hg-Te and Cd-Te of the rate of change of the liquidus temperature with respect to the Te concentration for Te mole fractions slightly above 0.5. The measured free volumes, the calculated atomic Te concentrations, the estimated temperature corrections for free-volume effects, and the corrected liquidus temperatures are summarized in Table 4.

Table 5 lists the liquidus and solidus temperatures determined in this investigation. Table 5 also gives the corrected \( x \)-values based on \( x = \frac{n_{\text{Cd}}}{(n_{\text{Cd}} + n_{\text{Hg}})} \). The phase diagram data are plotted in Figure 8.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( n_{\text{Cd}} ) (cm(^3))</th>
<th>( n_{\text{Hg}} ) (cm(^3))</th>
<th>( n_{\text{Te}} ) (cm(^3))</th>
<th>( x )</th>
<th>( x ) (correction)</th>
<th>( x ) (temperature)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.19</td>
<td>0.26</td>
<td>0.69</td>
<td>0.88</td>
<td>0.96</td>
<td>0.74</td>
</tr>
</tbody>
</table>

Table 4. Free-Volume Correction Parameters and Corrected Liquidus Temperatures.
TABLE 5. LIQUIDUS AND SOLIDUS TEMPERATURES FOR Hg$_{1-x}$Cd$_x$Te.

<table>
<thead>
<tr>
<th>Nominal composition (x)</th>
<th>Actual composition at solidus (x)</th>
<th>Solidus temperature (°C)</th>
<th>Actual composition at liquidus (x)</th>
<th>Liquidus temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.100</td>
<td>690</td>
<td>0.100</td>
<td>733</td>
</tr>
<tr>
<td>0.2</td>
<td>0.200</td>
<td>706</td>
<td>0.200</td>
<td>792</td>
</tr>
<tr>
<td>0.3</td>
<td>0.301</td>
<td>727</td>
<td>0.302</td>
<td>841</td>
</tr>
<tr>
<td>0.4</td>
<td>0.402</td>
<td>748</td>
<td>0.404</td>
<td>889</td>
</tr>
<tr>
<td>0.6</td>
<td>0.604</td>
<td>810</td>
<td>0.607</td>
<td>954</td>
</tr>
<tr>
<td>0.7</td>
<td>0.704</td>
<td>850</td>
<td>0.707</td>
<td>99</td>
</tr>
<tr>
<td>0.8</td>
<td>0.806</td>
<td>904</td>
<td>0.810</td>
<td>105</td>
</tr>
<tr>
<td>0.9</td>
<td>0.905</td>
<td>950</td>
<td>0.907</td>
<td>105</td>
</tr>
</tbody>
</table>

Figure 8. Hg$_{1-x}$Cd$_x$Te phase diagram.
2.4 Error Analysis and Comparison with Previous Results

The major recognized sources of error in the phase diagram data are the thermocouple calibrations, the subjectivity in selecting the proper phase-transformation points from the DTA curves, and the uncertainties in the ampule free-volume corrections.

Because the Sb melting point (630.7°C) was used to calibrate the thermocouples during each DTA run, the calibration should be quite accurate near that temperature and decrease in accuracy with increasing temperature. A type-K thermocouple calibrated at 630.7°C should be accurate to within ±2°C up to 930°C. The measured melting temperature of a Ag standard sample differed from the IPTS-68 value of 930°C by not more than ±3°C in tests of three different thermocouple combinations used during the course of this investigation. Therefore, the expression \(3(T - 631°C)/(930-631)\) was used as the calibration uncertainty at temperature T, which is equivalent to an uncertainty at the Ag melting point of 3.3°C and is considered adequate to include any graph-paper calibration errors as well as thermocouple calibration errors. For each sample, the calculated uncertainties arising from the temperature measurement uncertainties are listed in Table 6.

<table>
<thead>
<tr>
<th>TABLE 6. UNCERTAINTIES OF THE SOLIDUS AND LIQUIDUS TEMPERATURES.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solidus temperatures</strong></td>
</tr>
<tr>
<td>Composition (x)</td>
</tr>
<tr>
<td>0.1</td>
</tr>
<tr>
<td>0.2</td>
</tr>
<tr>
<td>0.3</td>
</tr>
<tr>
<td>0.4</td>
</tr>
<tr>
<td>0.6</td>
</tr>
<tr>
<td>0.7</td>
</tr>
<tr>
<td>0.8</td>
</tr>
<tr>
<td>0.9</td>
</tr>
</tbody>
</table>
The second source of error is in determination of the critical points of the DTA curves. For the solidus points, the extrapolation of the $S$ vs $T_s$ curve to the baseline for alloys with $0.1 < x < 0.7$ and the choice of the onset of deviation from the baseline for alloys with $x = 0.8$ or $0.9$ are somewhat subjective. Similarly, there were uncertainties in identifying the liquidus points. The latter uncertainties were about $10^\circ C$ except for the $x = 0.1$ sample, for which the liquidus onset occurred where the curve had a very steep slope, and for the $x = 0.8$ and $0.9$ samples, for which the sharpness of the liquidus onset was somewhat more rounded as shown in Figure 6. Estimates of subjectivity in reading the DTA curves are given in Table 6 under the columns headed "Reading DTA Curve."

The uncertainties listed for the free-volume corrections are $25\%$ of the total free-volume corrections.

The total uncertainties listed in Table 6 are the sums of the individual uncertainties and are believed to represent the maximum possible errors in the reported phase-equilibria temperatures.

The solidus and liquidus temperatures are compared with the results of previous investigations in Figure 9. The data of Ray and Spencer$^{17}$ and Blair and Newham$^{18}$ were derived from DTA measurements. Harman's$^{19}$ data are from chemical analyses of first-to-freeze regions of molten alloy samples. Steininger's$^{7}$ data were derived from thermal analyses of samples in a high-pressure apparatus.

A DTA measurement tends to yield too low a solidus temperature for a given $x$ because of possible inhomogeneities in the sample. The inherent error of the first-to-freeze method tends to yield too low an $x$ value for a given temperature. Therefore, on a temperature-composition plot, a solidus curve determined by the first-to-freeze compositions should fall at or above the true curve, and a solidus curve determined by DTA measurements should fall at or below the true curve. The present DTA data establish a solidus curve that nearly coincides with the lower limit of Harman's first-to-freeze data, and the two independent sets of data thus are corroborative.
For most compositions, the solidus and liquidus temperatures determined by this investigation are much larger than those reported by Ray and Spencer. A possible explanation for the discrepancies is advanced in Reference 20.

2.5 Liquid-Solid Equilibrium Parameters

The equilibria temperatures in Table 5 were used to calculate the temperature and composition dependence of the liquid/solid interface distribution coefficient, \( k(T) = \frac{x^S(T)}{x^L(T)} \), where \( x^S \) and \( x^L \) are the solidus and liquidus compositions, respectively. To facilitate the calculations, analytical expressions were developed for \( x^S(T)/x^L(T) \). Reasonably good fits to the phase diagram data were given by the following functional forms:

\[
x^S(T) = C_1 \sin \left( \frac{\pi}{2} T^* \right) + C_2 \sin \left( \frac{\pi}{2} T^{*1/2} \right) + C_3 \log_{10} \left( \frac{9T - 5618^\circ C}{412^\circ C} \right) + C_4 T^{*1/2}
\]

and
where $T^* = (T - 670^\circ C)/412^\circ C$ and the $C_i$ and $D_i$ are fitting constants. The values of the constants giving the best fits are given in Table 7. The solid curves drawn in Figures 8 and 9 are plots of Equations (10) and (11). The calculated values of $k(T)$ as functions of temperature and $x^S(T)$ are shown, respectively, in Figures 10 and 11. The failure of $k(T)$ to go through the point $(T, k) = (670^\circ C, 1)$ or the point $(x^S, k) = (0, 1)$ is an artifact of the solidus fit shown in Figure 8.

### TABLE 7. BEST VALUES FOR THE FITTING CONSTANTS $C_i$ AND $D_i$.  

<table>
<thead>
<tr>
<th>$i$</th>
<th>$C_i$</th>
<th>$D_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.380857</td>
<td>0.807640</td>
</tr>
<tr>
<td>2</td>
<td>0.086277</td>
<td>0.077209</td>
</tr>
<tr>
<td>3</td>
<td>1.200139</td>
<td>0.699767</td>
</tr>
<tr>
<td>4</td>
<td>-0.665231</td>
<td>-0.381693</td>
</tr>
</tbody>
</table>

Figure 10. Temperature dependence of the interface distribution coefficient.
To compare the observed DTA signals with those expected from the alloy properties, the equilibrium liquid fraction, \( M_L(T) \), was determined by using the lever rule, 
\[
M_L(T) = \left[ \frac{x_S(T) - x_0}{x_S(T) - x_L(T)} \right],
\]
and the analytical expressions of Equations (10) and (11) for \( x_S \) and \( x_L \). The temperature and composition dependences of \( M_L(T) \) are shown in Figure 12, and their temperature derivatives are shown in Figure 13. Figure 14 shows the observed normalized DTA signals for the various alloy compositions. A comparison of the results shown in Figure 14 with the results in Figure 13 shows a one-to-one correlation between the relative magnitudes of the DTA signals and the variation of \( dM_L/dT \) with composition. In principle, if the heat transfer characteristics of the furnace/sample system are well known, the compositional and temperature variations of \( dM_L/dT \) and thus \( M_L(x_S, x_L, x_0) \) can be calculated from the measured thermal arrest curves and vice versa. Approximate heat transfer calculations were performed, and in general, the calculated and observed DTA curves for the various alloy compositions were comparable. However, the detailed features of the calculated curves were sensitive to
small variations in the values of the heat transfer parameters, some of which are not precisely known. Meaningful deconvolutions of the measured DTA curves would require a precise thermal model for the sample/furnace system.

Figure 12. Temperature dependence of the alloy liquid fraction for various alloy compositions.
Figure 13. The temperature dependence of the rate of change with respect to temperature of the alloy liquid fraction for various alloy compositions.

Figure 14. Compositional variation of the observed DTA signals as functions of sample temperature.
3. PHASE EQUILIBRIA CALCULATIONS

Iterative phase-equilibria calculations, based on the regular associated solution (R.A.S.) theory\(^1,\)\(^2\) were performed, and a set of R.A.S. parameters was obtained by simultaneously least-squares-fitting the binary\(^3\)\(^-\)\(^6\) and pseudobinary phase diagrams. Using the set of R.A.S. parameters, the activities and partial pressures of Hg, Cd, and Te vapor over pseudobinary melts were calculated.

3.1 Theoretical Model

The term, regular solution, was used by Hildebrand\(^2\)\(^1\) to describe mixtures whose behavior was found experimentally to have certain regularities, and the definition of the term is essentially empirical. Subsequently, Guggenheim\(^2\)\(^2\) used the term to describe any mixture of molecules for which the entropy is that of an ideal solution but for which the interchange energy is not zero. The interchange energy is related to the nearest-neighbor pairwise interaction energies between atoms. Subsequently, Jordan\(^1\) considered the consequences of the association of type A and type B atoms in the liquid, i.e., the existence of AB species, and developed a thermodynamic description for such liquid solutions. He termed his formulation the regular associated solution (R.A.S.) theory. We assumed that the binary alloys Hg\(_{1-x}\)Te\(_x\) and Cd\(_{1-x}\)Te\(_x\), and hence the ternary Hg-Cd-Te alloys, are regular associated solutions, and used Jordan's formalism, as extended to ternary alloy systems by Szapiro,\(^2\) to determine the pertinent thermodynamic phase-equilibria parameters for the alloy system.

In the context of the R.A.S. theory, the liquidus and solidus ternary equations for an ABC ternary system are given by\(^2\):

\[
(1 - y) \exp \left[ \frac{W}{RT} y^2 \right] = \left( \frac{x_{AC}}{x_{AC}} \right)^{x_{AC}}
\]

\[
\times \exp \left[ \frac{\Delta H_1 + \omega x_2 (1 - 2x_1) + (\alpha_1 x_1 + \sigma_2 x_2 - 0.5 \alpha_1) (1 - 2x_3)}{RT} - \frac{\Delta S_1}{R} \right],
\]

(12)
and

\[
y \exp \left[ \frac{w}{RT} (1 - y^2) \right] = \frac{x_{BC}}{x_{BC}^*}
\]

\[
x \exp \left[ \frac{\Delta H_2 + \omega x_1 (1 - 2x_2) + (\alpha_1 x_1 + \alpha_2 x_2 - 0.5\alpha_2) (1 - 2x_3)}{RT} - \frac{\Delta S_2}{R} \right]
\]

where:

- \( y \) = mole fraction of complex BC in the solid phase,
- \( x_1, x_2, x_3 \) = atom fractions of A, B, and C, respectively,
- \( x_{AC}, x_{BC} \) = mole fractions of AC and BC in the liquid phase,
- \( T \) = absolute temperature,
- \( \Delta S_1, \Delta S_2 \) = entropies of fusion of the binary systems AC and BC,
- \( \Delta H_1, \Delta H_2 \) = heats of fusion of the binary systems AC and BC,
- \( R \) = the universal gas constant,
- \( \alpha_1 \) = the interaction parameter for the liquid binary system AC,
- \( \alpha_2 \) = the interaction parameter for the liquid binary system BC,
- \( \omega \) = the interaction parameter between species A and B,
- \( W \) = the interaction parameter between species AC and BC in the solid.

Asterisks denote the standard states of the liquid phases (stoichiometric compositions in the binary systems AC and BC). The interaction parameters \( \alpha_1, \alpha_2, \omega, \) and \( W \) are related to the interchange energies for the various pairwise interactions.

For the \( A_1-xC_x \) binary case, \( y = 0, x_2 = 0, \) and \( x_1 + x_3 = 1. \) Letting \( x = x_3, \) Equation (12) for this case reduces to

\[
\exp \left[ \frac{\Delta H_1 + 2\alpha (x - 0.5)^2}{RT} \right] = \frac{x_{AC}^*}{x_{AC}} \exp \left( -\frac{\Delta S_1}{R} \right)
\]

(14)
where
\[
x_{AC} = \frac{1 - (1 - 4(1 - x)x/(1 + \kappa))^1/2}{1 + [1 - 4(1 - x)x/(1 + \kappa)]^{1/2}},
\]
(15)
\[
x^* = \frac{x_{AC}}{x} \quad (x = 0.5),
\]
(16)
and \( \kappa \) is given in terms of the temperature-independent equilibrium constant, \( K \), by
\[
\kappa = K \exp \left( \frac{a}{2RT} \right) = \left( \frac{\beta^2}{1 - \beta^2} \right).
\]
(17)
The parameter \( \beta \) is defined by Equation (17) and is a measure of the degree of association in the liquid. For a completely associated solution, \( \kappa = 0 \), and thus \( \beta = 0 \). When the solution is completely dissociated, \( \kappa = \infty \) and \( \beta = 1 \). The activities of the species \( a_A \) and \( a_C \) for the binary melt are given by
\[
a_A = x_A \gamma_A = x_A \exp \left[ \frac{x^2 \alpha}{RT} \right],
\]
(18)
and
\[
a_C = x_C \gamma_C = x_C \exp \left[ \frac{(1 - x)^2 \alpha}{RT} \right],
\]
(19)
where \( \gamma_A \) and \( \gamma_C \) are the activity coefficients,
\[
x_A = x_1 [1 + x_{AC}] - x_{AC},
\]
(20)
and
\[
x_C = x_3 [1 + x_{AC}] - x_{AC}.
\]
(21)
For the pseudobinary cut, \( x_3 = 0.5 = x_1 + x_2 \), so that Equations (12) and (13) become
\[
(1 - y) \exp \left[ \frac{\omega}{RT} y^2 \right] = \frac{x_{AC}}{x_{AC}^*} \exp \left[ \frac{\Delta H_1 + \omega x_2(1 - 2x_1)}{RT} - \frac{\Delta S_1}{R} \right]
\]
(22)
and

\[
y \exp \left[ \frac{W}{RT} (1 - y)^2 \right] = \frac{x_{BC}^*}{x_{BC}} \exp \left[ \frac{\Delta H_2 + \omega x_1 (1 - 2x_2) - \Delta S_2}{RT} - \frac{\Delta S_2}{R} \right],
\]

where

\[
x_{AC} = \frac{x_1 x_C (1 + \sigma)}{\kappa_1 + x_C},
\]

\[
x_{BC} = \frac{x_2 x_C (1 + \sigma)}{\kappa_2 + x_C},
\]

and \( \sigma (\equiv x_{AC} + x_{BC}) \) is the solution of the cubic equation

\[
\frac{x_1}{\kappa_1 + 0.5 (1 - \sigma)} + \frac{x_2}{\kappa_2 + 0.5 (1 - \sigma)} = \frac{\sigma}{0.5 (1 - \sigma^2)}.
\]

The parameters \( \kappa_1(AC) \) and \( \kappa_2(BC) \) are defined by Equation (17), and the parameters \( x_{AC}^* \) \( (i = A, B) \) are defined by Equation (16).

The activities \( a_A, a_B, \) and \( a_C \) for the pseudobinary melt are given by the expressions:

\[
a_A = x_A \gamma_A = [x_1 (1 + x_{AC} + x_{BC}) - x_{AC}] \gamma_A^*
\]

\[
a_B = x_B \gamma_B = [x_2 (1 + x_{AC} + x_{BC}) - x_{BC}] \gamma_B^*
\]

and

\[
a_C = x_C \gamma_C = 0.5 [1 - x_{AC} - x_{BC}] \gamma_C,
\]

where \( \gamma_A, \gamma_B, \) and \( \gamma_C \) are the activity coefficients given by

\[
\gamma_A = \exp \left[ \frac{\omega x_2^2 + 0.25 \alpha_1 + (\omega + \alpha_1 - \alpha_2) (0.5 x_2)}{RT} \right],
\]

\[
\gamma_B = \exp \left[ \frac{\omega x_1^2 + 0.25 \alpha_2 + (\omega - \alpha_1 + \alpha_2) (0.5 x_1)}{RT} \right],
\]
and

\[
Y_C = \exp \left[ \frac{\alpha_1 x_1^2 + \alpha_2 x_2^2 + (\alpha_1 + \alpha_2 - \omega) x_1 x_2}{RT} \right].
\]  

(32)

3.2 Regular Associated Solution Parameters for the HgCdTe Alloy System

The R.A.S. parameters \( \alpha_1, \alpha_2, \beta_1, \beta_2, \omega, \) and \( \omega \) for the HgCdTe alloy system were determined by simultaneously least-squares-fitting the metal-rich segments of the binary liquidus curves and the pseudobinary (Figure 8) phase diagram. To facilitate the computations, Equations (22) and (23) were rewritten in the following forms:

\[
T = \frac{\Delta H_1 + \omega x_2 (1 - 2x_1) - \omega y^2}{R \left[ \ln(1 - y) - \ln \frac{x_{AC}}{x_{AC}^*} \right] + \Delta S_1} = T_2
\]

(33)

and

\[
T = \frac{\Delta H_2 + \omega x_1 (1 - 2x_2) - \omega (1 - y)^2}{R \left[ \ln y - \ln \frac{x_{BC}}{x_{BC}^*} \right] + \Delta S_2}
\]

(34)

These equations and Equation (14) were then fitted to the experimental data to obtain the best values of the parameters by minimizing the sum:

\[
S = \sum \left[ \left( \frac{\text{CdTe}}{T_1(c)} - \frac{\text{CdTe}}{T_1(e)} \right)^2 + \left( \frac{\text{HgTe}}{T_1(c)} - \frac{\text{HgTe}}{T_1(e)} \right)^2 \right.
\]

\[
+ \left( \frac{\text{HgCdTe}}{T_3(c)} - \frac{\text{HgCdTe}}{T_3(e)} \right)^2 + \left( \frac{\text{HgCdTe}}{T_2(c)} - \frac{\text{HgCdTe}}{T_2(e)} \right)^2 \right].
\]

(35)
The symbols c and e designate, respectively, the calculated and experimental values.

Table 8 lists the calculated values of the parameters as well as the pertinent thermodynamic quantities used in the calculations. Table 9 indicates the relative accuracy of the fit to the measured pseudobinary data. The calculated mole fractions of the various species and complexes as functions of the solidus temperature are given in Table 10 to illustrate the relative effects of association on the Hg$_1$–Cd$_x$Te solutions.

**TABLE 8. R.A.S. PARAMETERS AND THERMODYNAMIC DATA FOR THE Hg-Cd-Te SYSTEM.**

<table>
<thead>
<tr>
<th>R.A.S. parameters</th>
<th>Thermodynamic data</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_1 = 0.9716$</td>
<td>$\Delta S_1 = 9.2$ e.u. = 38.5 J/mol K$^{(a)}$</td>
</tr>
<tr>
<td>$\alpha_1 = 953.0$ cal/mol = 3.987 kJ/mol</td>
<td>$\Delta S_2 = 8.9$ e.u. = 37.2 J/mol K$^{(a)}$</td>
</tr>
<tr>
<td>$K_2 = 0.1201$</td>
<td>$\Delta H_1 = 8675.6$ cal/mol = 36.299 kJ/mol</td>
</tr>
<tr>
<td>$\alpha_2 = 9051$ cal/mol = 37.87 kJ/mol</td>
<td>$\Delta H_2 = 12012$ cal/mol = 50.258 kJ/mol</td>
</tr>
<tr>
<td>$\omega = 971.7$ cal/mol = 4.066 kJ/mol</td>
<td>$T_{f1} = 943$ K$^{(a)}$</td>
</tr>
<tr>
<td>$W = 836.0$ cal/mol = 3.498 kJ/mol</td>
<td>$T_{f2} = 1365$ K$^{(a)}$</td>
</tr>
</tbody>
</table>

$^{(a)}$A. Laugier, Revue de Physique Appliquée 8, 259 (1973).

(b) The subscript 1 refers to HgTe and the subscript 2 refers to CdTe.
TABLE 9. A COMPARISON OF EXPERIMENTAL AND CALCULATED TEMPERATURES FOR Hg\(_{1-x}\)Cd\(_x\)Te.

<table>
<thead>
<tr>
<th>(T_{\text{exp}}) (K)</th>
<th>(T_2^\dagger) (K)</th>
<th>(T_3^\dagger) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>973</td>
<td>968</td>
<td>981</td>
</tr>
<tr>
<td>998</td>
<td>991</td>
<td>1003</td>
</tr>
<tr>
<td>1023</td>
<td>1012</td>
<td>1026</td>
</tr>
<tr>
<td>1048</td>
<td>1032</td>
<td>1052</td>
</tr>
<tr>
<td>1073</td>
<td>1053</td>
<td>1074</td>
</tr>
<tr>
<td>1098</td>
<td>1074</td>
<td>1098</td>
</tr>
<tr>
<td>1123</td>
<td>1097</td>
<td>1122</td>
</tr>
<tr>
<td>1148</td>
<td>1121</td>
<td>1145</td>
</tr>
<tr>
<td>1173</td>
<td>1149</td>
<td>1168</td>
</tr>
<tr>
<td>1198</td>
<td>1180</td>
<td>1192</td>
</tr>
<tr>
<td>1223</td>
<td>1213</td>
<td>1217</td>
</tr>
<tr>
<td>1248</td>
<td>1254</td>
<td>1242</td>
</tr>
<tr>
<td>1273</td>
<td>1298</td>
<td>1268</td>
</tr>
<tr>
<td>1298</td>
<td>1358</td>
<td>1294</td>
</tr>
</tbody>
</table>

The quantities designated by \(\dagger\) were calculated using Equations (33) and (34); the parameters are given in Table 8.

TABLE 10. MOLE FRACTIONS OF SPECIES IN LIQUID PHASE AS FUNCTIONS OF LIQUIDUS TEMPERATURE.

<table>
<thead>
<tr>
<th>(T_L) (K)</th>
<th>(x_{\text{Hg}})</th>
<th>(x_{\text{Cd}})</th>
<th>(x_{\text{Te}})</th>
<th>(x_{\text{HgTe}})</th>
<th>(x_{\text{CdTe}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>973</td>
<td>0.387</td>
<td>0.001</td>
<td>0.388</td>
<td>0.198</td>
<td>0.026</td>
</tr>
<tr>
<td>998</td>
<td>0.379</td>
<td>0.002</td>
<td>0.380</td>
<td>0.189</td>
<td>0.050</td>
</tr>
<tr>
<td>1023</td>
<td>0.370</td>
<td>0.003</td>
<td>0.373</td>
<td>0.179</td>
<td>0.075</td>
</tr>
<tr>
<td>1048</td>
<td>0.359</td>
<td>0.004</td>
<td>0.363</td>
<td>0.169</td>
<td>0.104</td>
</tr>
<tr>
<td>1073</td>
<td>0.348</td>
<td>0.005</td>
<td>0.354</td>
<td>0.158</td>
<td>0.134</td>
</tr>
<tr>
<td>1098</td>
<td>0.335</td>
<td>0.007</td>
<td>0.342</td>
<td>0.147</td>
<td>0.169</td>
</tr>
<tr>
<td>1123</td>
<td>0.319</td>
<td>0.010</td>
<td>0.329</td>
<td>0.134</td>
<td>0.207</td>
</tr>
<tr>
<td>1148</td>
<td>0.302</td>
<td>0.013</td>
<td>0.315</td>
<td>0.120</td>
<td>0.250</td>
</tr>
<tr>
<td>1173</td>
<td>0.282</td>
<td>0.017</td>
<td>0.299</td>
<td>0.106</td>
<td>0.296</td>
</tr>
<tr>
<td>1198</td>
<td>0.268</td>
<td>0.022</td>
<td>0.281</td>
<td>0.091</td>
<td>0.348</td>
</tr>
<tr>
<td>1223</td>
<td>0.231</td>
<td>0.029</td>
<td>0.260</td>
<td>0.075</td>
<td>0.405</td>
</tr>
<tr>
<td>1248</td>
<td>0.200</td>
<td>0.038</td>
<td>0.238</td>
<td>0.059</td>
<td>0.465</td>
</tr>
<tr>
<td>1273</td>
<td>0.164</td>
<td>0.050</td>
<td>0.214</td>
<td>0.044</td>
<td>0.529</td>
</tr>
<tr>
<td>1298</td>
<td>0.121</td>
<td>0.066</td>
<td>0.187</td>
<td>0.028</td>
<td>0.587</td>
</tr>
</tbody>
</table>
3.3 Component Partial Pressures over the Pseudobinary Melt

Following Jordan,\textsuperscript{23} the partial pressures of the components over the pseudobinary melt can be related to the activities by the expressions

\begin{align*}
P_{\text{Hg}} &= a_{\text{Hg}} P_{\text{Hg}}^0, \quad (36) \\
P_{\text{Cd}} &= a_{\text{Cd}} P_{\text{Cd}}^0, \quad (37)
\end{align*}

and

\[ P_{\text{Te}_2} = a_{\text{Te}}^2 P_{\text{Te}_2}^0, \quad (38) \]

where \( P_{\text{Hg}}^0 \), \( P_{\text{Cd}}^0 \), and \( P_{\text{Te}_2}^0 \) are the vapor pressures over the standard states and the respective activities \( a_{\text{Hg}} \), \( a_{\text{Cd}} \), and \( a_{\text{Te}} \) are given by Equations (27-29). Using Equations (36-38) and the parameters of Table 8, the component partial pressures were calculated as functions of the liquidus temperature, and the results are summarized in Table 11 and Figure 15. Figure 16 illustrates the temperature variation of the Hg partial pressure over the pseudobinary melt as a function of the Cd fraction. The calculated Hg partial pressures are in reasonable agreement with Steininger's experimental results.\textsuperscript{7} However, the validity of the calculated R.A.S. parameters values and thus the calculated partial pressures are sensitively dependent upon assumptions concerning the melt composition. For example, the derivation of Equations (12) and (13) assumes negligible Hg-Hg, Cd-Cd, and Te-Te associations in the melt. The validity of at least the last of the assumptions is highly suspect.
TABLE 11. CALCULATED COMPONENT PARTIAL PRESSURES OVER THE
Hg$_{1-x}$Cd$_x$Te MELT AT THE LIQUIDUS TEMPERATURE.

<table>
<thead>
<tr>
<th>(T_L) (K)</th>
<th>Composition (a)</th>
<th>(a_{\text{Hg}})</th>
<th>(a_{\text{Cd}})</th>
<th>(a_{\text{Te}})</th>
<th>(p_o(a)) $\text{Hg}_0$ (atm)</th>
<th>(p_o(b)) $\text{Cd}_0$ (atm)</th>
<th>(p_o(c)) $\text{Te}_2$ (atm)</th>
<th>(p_{\text{Hg}}) (atm)</th>
<th>(p_{\text{Cd}}) (atm)</th>
<th>(p_{\text{Te}_2}) (atm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>973.2</td>
<td>0.044</td>
<td>0.421</td>
<td>0.009</td>
<td>0.457</td>
<td>50.6</td>
<td>0.457</td>
<td>0.039</td>
<td>21.3 (17.5)</td>
<td>0.004</td>
<td>0.008</td>
</tr>
<tr>
<td>998.2</td>
<td>0.084</td>
<td>0.396</td>
<td>0.016</td>
<td>0.463</td>
<td>60.8</td>
<td>0.626</td>
<td>0.056</td>
<td>24.1 (21.0)</td>
<td>0.010</td>
<td>0.012</td>
</tr>
<tr>
<td>1023.2</td>
<td>0.124</td>
<td>0.374</td>
<td>0.023</td>
<td>0.468</td>
<td>72.5</td>
<td>0.844</td>
<td>0.078</td>
<td>27.1 (25.0)</td>
<td>0.020</td>
<td>0.017</td>
</tr>
<tr>
<td>1048.2</td>
<td>0.170</td>
<td>0.350</td>
<td>0.031</td>
<td>0.473</td>
<td>85.6</td>
<td>1.120</td>
<td>0.108</td>
<td>29.9 (29.5)</td>
<td>0.035</td>
<td>0.024</td>
</tr>
<tr>
<td>1073.2</td>
<td>0.216</td>
<td>0.327</td>
<td>0.039</td>
<td>0.476</td>
<td>100.6</td>
<td>1.470</td>
<td>0.146</td>
<td>32.8 (34.5)</td>
<td>0.057</td>
<td>0.033</td>
</tr>
<tr>
<td>1098.2</td>
<td>0.268</td>
<td>0.302</td>
<td>0.048</td>
<td>0.479</td>
<td>117.0</td>
<td>1.910</td>
<td>0.196</td>
<td>35.3 (40.4)</td>
<td>0.091</td>
<td>0.041</td>
</tr>
<tr>
<td>1123.2</td>
<td>0.324</td>
<td>0.278</td>
<td>0.057</td>
<td>0.480</td>
<td>135.0</td>
<td>2.440</td>
<td>0.259</td>
<td>37.5 (47.0)</td>
<td>0.140</td>
<td>0.061</td>
</tr>
<tr>
<td>1148.2</td>
<td>0.384</td>
<td>0.252</td>
<td>0.068</td>
<td>0.479</td>
<td>155.0</td>
<td>3.090</td>
<td>0.338</td>
<td>39.1 (53.5)</td>
<td>0.210</td>
<td>0.078</td>
</tr>
<tr>
<td>1173.2</td>
<td>0.446</td>
<td>0.227</td>
<td>0.080</td>
<td>0.475</td>
<td>177.0</td>
<td>3.880</td>
<td>0.436</td>
<td>40.1 (61.0)</td>
<td>0.309</td>
<td>0.098</td>
</tr>
<tr>
<td>1198.2</td>
<td>0.514</td>
<td>0.200</td>
<td>0.094</td>
<td>0.468</td>
<td>201.0</td>
<td>4.820</td>
<td>0.556</td>
<td>40.2 (69.0)</td>
<td>0.451</td>
<td>0.122</td>
</tr>
<tr>
<td>1223.2</td>
<td>0.586</td>
<td>0.172</td>
<td>0.110</td>
<td>0.456</td>
<td>227.0</td>
<td>5.930</td>
<td>0.703</td>
<td>39.0 (55.0)</td>
<td>0.654</td>
<td>0.146</td>
</tr>
<tr>
<td>1248.2</td>
<td>0.660</td>
<td>0.143</td>
<td>0.130</td>
<td>0.439</td>
<td>256.0</td>
<td>7.250</td>
<td>0.880</td>
<td>36.5</td>
<td>0.943</td>
<td>0.170</td>
</tr>
<tr>
<td>1273.2</td>
<td>0.736</td>
<td>0.113</td>
<td>0.155</td>
<td>0.415</td>
<td>286.0</td>
<td>8.780</td>
<td>1.090</td>
<td>32.3</td>
<td>1.360</td>
<td>0.188</td>
</tr>
<tr>
<td>1298.2</td>
<td>0.816</td>
<td>0.081</td>
<td>0.188</td>
<td>0.385</td>
<td>318.0</td>
<td>10.600</td>
<td>1.340</td>
<td>25.7</td>
<td>1.980</td>
<td>0.199</td>
</tr>
</tbody>
</table>

Values in parentheses correspond to Steen's experimental results (Ref. 7).

\(p_o\) represent the vapor pressures over the elemental melts. \(p_{\text{Hg}}\), \(p_{\text{Cd}}\) and \(p_{\text{Te}_2}\) represent the vapor pressures over the elemental melts.

(a) \(p_o\) was obtained from the equation, \(\log_{10} p_o = 4.89 - \frac{3080}{T/(K)}\), which gives an accuracy of better than 1% (S. Sugawa and others, Bull. Jap. Soc. Mech. Eng., 5, 711 (1962)).

(b) \(p_o\) was obtained from the equation, \(\log_{10} p_o = 5.105 - \frac{5300}{T/(K)}\), which gives an accuracy of better than 0.5% (D.R. Stull and G.E. Simko, Thermodynamic Properties of the Elements. Academic Press, New York, 1963).  

(c) \(p_o\) was obtained from the equation, \(\log_{10} p_o = 4.719 - \frac{5960}{T/(K)}\), which gives an accuracy of better than 0.5% (A.N. Nesmeyanov, Vapor Pressure of the Elements. Academic Press, New York, 1963).
Figure 15. Component partial pressures over the Hg$_{1-x}$Cd$_x$Te melt.
Figure 16. The temperature variation of Hg partial pressure over the $\text{Hg}_1-x\text{Cd}_x\text{Te}$ melt as a function of Cd fraction.
4. HIGH-TEMPERATURE-GRADIENT DIRECTIONAL SOLIDIFICATION

4.1 Alloy Preparation

Hg_{0.8}Cd_{0.2}Te alloys were prepared by reacting 99.9999% pure elemental constituents in sealed, evacuated, fused-quartz tubing. The tubing dimensions were 5-mm i.d. x 10-mm o.d. To prepare an ampule, the end of the tubing where solidification was to begin was tapered to a point to enhance the probability of single-crystal growth. For the initial experiments, a 5-mm i.d. x 10-mm o.d. quartz tube was fused to the tapered end of the ampule to serve as a coupling sleeve to a 5-mm diam quartz-rod pedestal, which supported the ampule during the growth process. This coupling arrangement was susceptible to mechanical failure, and after several failures, a configuration was used in which a 4-mm diameter silica rod is fused directly to the tapered end of the ampule. The solid silica rod inserts into a 5-mm i.d. silica tube, which serves as a pedestal.

Following fabrication, the ampules were cleaned thoroughly, with the final cleaning being done with a dilute HF solution, evacuated, and baked at 1150°C. The ampules were loaded with precisely weighed amounts of Hg, Cd, and Te. Following loading, the ampules were sealed and the alloys were cast as described in Section 2.1.

Altogether, 12 crystal-growth ampules (L1-L12) containing alloys with x = 0.2 were prepared. The ampules L1-L5 contained stoichiometric proportions of the constituent elements. The alloy preparations yielded highly p-type ingots because of the Te excess in the melt caused by the preferential Hg evaporation into the ampule free volume. For ampules L6-L12, excess mercury was added to compensate for the preferential mercury evaporation. Ampules L1, L2, and L8 failed during casting. Ampules L9, L10, and L11 showed wetting of the ampule wall by the alloy, and they were discarded.

4.2 Experimental Arrangement and Procedures for Unidirectional Crystal Growth

The precast alloys were regrown by unidirectional solidification in the growth apparatus illustrated in Figure 17. The ampule is mounted, with its tapered end down, atop a quartz pedestal and remains stationary during the growth process. Two resistively heated, tubular furnaces provide for the
temperature control of the hot and cold zones. The furnace assembly travels upward on vertical ways so that the crystal grows progressively upward from the bottom, tapered end of the ampule. Each furnace is provided with a heat-pipe isothermal furnace liner to provide two well-defined heated zones. The hot-zone heat-pipe is sodium-charged, and the cold-zone heat-pipe is either sodium or mercury charged depending on the temperature requirements. The heat-pipes are separated by a heat barrier. Besides providing the necessary thermal isolation between the heated zones, the barrier also provides a semi-
adiabatic region. The barrier consists of 4-mm thick zirconia-felt or various thicknesses of fire-brick disks sandwiched between two 25-μm thick polished platinum foils on the hot side and two 25-μm aluminum foils on the cold side. The diameter of the circular opening in the heat barrier is 12-mm to accept 10-mm diameter ampules.

Prior to a given growth run, a dummy ampule with an attached thermocouple is placed in the upper zone of the furnace, and the two heated-zone temperatures are raised to their desired values. The furnace assembly is translated upward, and the thermocouple output is recorded as a function of furnace position to establish the temperature variation along the furnace assembly axis. The furnaces are then cooled to ambient temperature, the growth ampule is positioned in the upper zone, and the zone temperatures are increased to the previous values. Prior to growth initiation, the molten alloy is maintained at temperature for 24 h to assure melt homogenization.

4.3 Bridgman Crystal Growth Runs

Crystal growth runs were completed for ampules L3, L4, L5, L6, and L7 at furnace translation rates of 0.597, 1.12, 5.62, 0.310, and 0.068 μm/s, respectively. The longitudinal temperature profiles in the furnace at the initiation of growth of ingots L3 and L4 are shown in Figures 18 and 19, respectively, and the furnace profile for ingots L6 and L7 is shown in Figure 20.

The recrystallized ingots were removed from the ampules by dissolving the quartz in concentrated HF. Sample L5 showed excessive wetting between the ampule and the ingot and was not evaluated further. The remaining ingots were sliced into wafers by a wire saw for characterization.
Figure 18. Temperature profile of crystal-growth furnace during growth of ingot L3.
Figure 19. Temperature profile of crystal-growth furnace during growth of ingot L4.

Figure 20. Temperature profile of crystal-growth furnace during growth of ingots L6 and L7.
4.4 Ingot Characterization

4.4.1 Determination of Alloy Composition by Mass Density Measurements

The crystal lattice spacing of the Hg$_{1-x}$Cd$_x$Te alloys varies so little with x that its measurement cannot be used readily to calculate precise values for the compositions of specimens. For this study, the average x-values of slices transverse to the growth axis were calculated from the measured mass densities and values of the crystal lattice constant published by Woolley and Ray.\(^\text{24}\)

The lattice constant data of Woolley and Ray can be represented by the cubic equation

\[ a_o = 0.646153 + (0.73671 x + 1.90501 x^2 - 0.69347 x^3)/1000, \] (39)

where \(a_o\) is the cubic lattice constant in nanometers and x is the mole fraction of CdTe in the Hg$_{1-x}$Cd$_x$Te alloy. There are, on the average, 4x Cd atoms, 4(1-x) Hg atoms, and 4 Te atoms in each cubic unit cell. Thus, the lattice constant is related to the mass density, \(\rho_m\), by the expression

\[ a_o = \left[ \frac{4x M_{Cd} + 4(1-x) M_{Hg} + 4 M_{Te}}{\rho_m} \right]^{1/3}, \] (40)

where \(M_{Cd}\), \(M_{Hg}\), and \(M_{Te}\) are the atomic masses of Cd, Hg, and Te, respectively. For a given density, the value of x can be determined by simultaneously solving Equations (39) and (40).

The mass density of a specimen was determined by obtaining its weight, \(W_a\), in air and its weight, \(W_w\), when it is immersed in water. The specimen density is given by the relation

\[ \rho_m = \frac{W_a \rho_w - W_w \rho_a}{W_a - W_w}, \] (41)

where \(\rho_w\) is the mass density of water and \(\rho_a\) is the mass density of air.
Near $x = 0.2$, an uncertainty of $0.0022 \text{ g/cm}^3$ in $\rho_m$ leads to an uncertainty of about $0.001$ in calculating $x$. The uncertainty in $\rho_m$ can be approximated by

$$\Delta \rho_m = \frac{(\rho_m + \rho_w) \Delta w_a + \rho_m \Delta w_w + \Delta w_a \Delta \rho_w}{w_a - w_w}, \tag{42}$$

where $\Delta w_a$, $\Delta w_w$, and $\Delta \rho_w$ are the uncertainties in $w_a$, $w_w$, and $\rho_w$, respectively. Because $\Delta w_a$ and $\Delta \rho_w$ are usually much smaller than $\Delta w_w$,

$$\Delta \rho_m = \frac{\rho_m \Delta w_w}{w_a - w_w} = \frac{\rho_m^2 \Delta w_w}{w_a \rho_w} = \frac{\rho_m^2 \Delta W_w}{w_a}. \tag{43}$$

The uncertainty in $x$, $\Delta x$, is thus given by

$$\Delta x = \frac{\Delta W_w \rho_m^2}{2.2 \ w_a}, \tag{44}$$

where the density is in the units of $\text{g/cm}^3$. For specimens that weigh about 0.5 g, $\Delta W_w$ must be less than 0.00002 g to give $x$ to within $\pm 0.001$.

The method described by Bowman and Schooner\textsuperscript{25} was used for the mass density determinations. The $\text{Hg}_1-x\text{Cd}_x\text{Te}$ specimen is immersed in water, and the water is boiled briefly to eliminate gases dissolved in the water and to rid the specimen of minute air bubbles that may be sorbed. After the sample and the water have cooled to room temperature, the weight of the immersed specimen is measured with a balance that weighs with a precision of $\pm 0.000001$ g. However, the precision of the weight determination in water is much poorer than this because of the surface-tension forces upon the 0.013-mm diam wire that is used to suspend the specimen from the balance arm. Some of the suspension wires that were prepared permitted the weight in water to be determined with an accuracy of $\pm 0.00001$ g, but usually an accuracy of only $\pm 0.00002$ g is achieved. To do significantly better requires an inordinate amount of time.
The following expression, from Reference 22, was used to calculate the density of the water in which the sample is immersed:

\[
\rho_w = \left[ \frac{(t_w - 3.9863) \times 2}{508929.2} + \frac{t_w + 288.9414}{t_w + 68.12963} \right] \times 0.999973 \times \left[ \frac{1}{1 - C} \times \left( \frac{1}{101325} + \frac{B}{10330} - 1 \right) \right] \times \left[ 1 - (2.11 - 0.053t_w) \left( 1 - \frac{1}{1 + D} \right) \times 10^{-6} \right] \text{g/cm}^3.
\]

In this expression, \( t_w \) is the water temperature in \(^{\circ}\text{C} \), \( C \) is the compressibility of water (\( C = 471 \times 10^{-12} \text{ Pa}^{-1} \)), \( B \) is the barometric pressure in Pa, \( I \) is the depth of immersion of the sample in water in mm, and \( D \) is the number of days elapsed since the water was boiled. After the measurement in water, the specimen is dried and weighed in air with the same balance. The mass density of air is calculated from the following expression given in Reference 25:

\[
\rho_a = \left[ \frac{464.568 - H(0.085594t_a^2 - 1.8504t_a + 34.47)}{t_a + 273.16} \times 10^{-6} \right] \text{g/cm}^3,
\]

where \( H \) is the relative humidity in percent and \( t_a \) is the air temperature in \(^{\circ}\text{C} \).

Nichrome (80Ni-20Cr) wire, 0.013 mm in diam, was used to suspend the specimens for the weighings in water. The wires were baked at 700-800\(^{\circ}\text{C} \) for 1 h in air at 0.1 Pa (1 x 10\(^{-3}\) Torr) to prepare their surfaces. The oxidized surfaces of the wires developed microfissures when the wires were cooled. These microfissures cause the water meniscus and surface tension to be nearly the same at each point along the wire when it is raised and lowered in the water during the weighings. No surface film on the water is tolerable, and microscopic dust particles in the meniscus region can invalidate the weight measurements in water.
Tables 12, 13, and 14 summarize the results of mass density measurements for ingots L3, L4, and L6. The distance from the tip given in the tables is the distance to the midplane of a slice.

**TABLE 12. AVERAGE ALLOY COMPOSITIONS FOR VARIOUS POSITIONS ALONG THE AXIS OF INGOT L3.**

<table>
<thead>
<tr>
<th>Sample number</th>
<th>Distance from tip (cm)</th>
<th>Mass density (g/cm³)</th>
<th>Average composition (x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L31</td>
<td>0.25</td>
<td>7.0319</td>
<td>0.472</td>
</tr>
<tr>
<td>L32</td>
<td>0.64</td>
<td>7.2416</td>
<td>0.378</td>
</tr>
<tr>
<td>L35</td>
<td>2.07</td>
<td>7.5906</td>
<td>0.221</td>
</tr>
<tr>
<td>L310</td>
<td>5.01</td>
<td>7.6312</td>
<td>0.203</td>
</tr>
<tr>
<td>L312</td>
<td>6.35</td>
<td>7.6237</td>
<td>0.207</td>
</tr>
<tr>
<td>L313</td>
<td>7.27</td>
<td>7.6296</td>
<td>0.204</td>
</tr>
<tr>
<td>L314</td>
<td>8.22</td>
<td>7.6285</td>
<td>0.204</td>
</tr>
<tr>
<td>L321</td>
<td>12.60</td>
<td>7.6328</td>
<td>0.202</td>
</tr>
<tr>
<td>L322</td>
<td>13.32</td>
<td>7.6377</td>
<td>0.200</td>
</tr>
<tr>
<td>L327</td>
<td>15.91</td>
<td>7.7200</td>
<td>0.163</td>
</tr>
<tr>
<td>L328</td>
<td>16.60</td>
<td>7.8468</td>
<td>0.106</td>
</tr>
</tbody>
</table>
### TABLE 13. AVERAGE ALLOY COMPOSITIONS FOR VARIOUS POSITIONS ALONG THE AXIS OF INGOT L4.

<table>
<thead>
<tr>
<th>Sample number</th>
<th>Distance from tip (cm)</th>
<th>Mass density (g/cm³)</th>
<th>Average composition (x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L41T</td>
<td>0.29</td>
<td>7.1098</td>
<td>0.437</td>
</tr>
<tr>
<td>L41A</td>
<td>0.73</td>
<td>7.4947</td>
<td>0.265</td>
</tr>
<tr>
<td>L41B</td>
<td>0.81</td>
<td>7.5886</td>
<td>0.222</td>
</tr>
<tr>
<td>L41C</td>
<td>1.26</td>
<td>7.6051</td>
<td>0.215</td>
</tr>
<tr>
<td>L41D</td>
<td>1.53</td>
<td>7.6144</td>
<td>0.211</td>
</tr>
<tr>
<td>L41E</td>
<td>1.79</td>
<td>7.6220</td>
<td>0.207</td>
</tr>
<tr>
<td>L41G</td>
<td>2.33</td>
<td>7.6174</td>
<td>0.209</td>
</tr>
<tr>
<td>L41I</td>
<td>2.86</td>
<td>7.6176</td>
<td>0.209</td>
</tr>
<tr>
<td>L41K</td>
<td>3.39</td>
<td>7.6194</td>
<td>0.208</td>
</tr>
<tr>
<td>L42</td>
<td>4.32</td>
<td>7.6252</td>
<td>0.206</td>
</tr>
<tr>
<td>L43</td>
<td>5.40</td>
<td>7.6162</td>
<td>0.210</td>
</tr>
<tr>
<td>L44</td>
<td>6.43</td>
<td>7.6211</td>
<td>0.208</td>
</tr>
<tr>
<td>L45</td>
<td>7.45</td>
<td>7.6334</td>
<td>0.202</td>
</tr>
<tr>
<td>L46</td>
<td>8.47</td>
<td>7.6404</td>
<td>0.199</td>
</tr>
<tr>
<td>L47</td>
<td>9.49</td>
<td>7.6327</td>
<td>0.202</td>
</tr>
<tr>
<td>L48</td>
<td>10.52</td>
<td>7.6320</td>
<td>0.203</td>
</tr>
<tr>
<td>L49</td>
<td>11.54</td>
<td>7.6206</td>
<td>0.208</td>
</tr>
<tr>
<td>L410</td>
<td>12.32</td>
<td>7.6154</td>
<td>0.210</td>
</tr>
<tr>
<td>L411A</td>
<td>13.07</td>
<td>7.6171</td>
<td>0.210</td>
</tr>
<tr>
<td>L411B</td>
<td>13.33</td>
<td>7.6263</td>
<td>0.205</td>
</tr>
<tr>
<td>L411D</td>
<td>13.87</td>
<td>7.6474</td>
<td>0.196</td>
</tr>
<tr>
<td>L411F</td>
<td>14.40</td>
<td>7.6976</td>
<td>0.173</td>
</tr>
<tr>
<td>L411G</td>
<td>14.67</td>
<td>7.7458</td>
<td>0.151</td>
</tr>
<tr>
<td>L411H</td>
<td>14.93</td>
<td>7.8229</td>
<td>0.117</td>
</tr>
<tr>
<td>L411J</td>
<td>15.21</td>
<td>8.0653</td>
<td>0.007</td>
</tr>
</tbody>
</table>
4.4.2 Infrared Transmission Measurements

From ingots L3, L4, and L6, thin (~200-300 μm) slices were prepared for evaluation of the radial compositional variation by infrared transmission-edge mapping. The transmission measurements were made at room temperature through 1-mm diam areas at regularly spaced locations on a slice.

The initial measurements on slices from ingots L3 and L4 showed no infrared (IR) transmission. Subsequently, the thicknesses of these slices were reduced to 20-50 μm by polishing and etching, and the measurements were repeated. However, even for these small thicknesses, the slices remained essentially opaque to IR radiation. This result was attributed to the highly p-type character of the slices.

The slices from ingot L6 showed up to 40% transmission above the cut-off wavelengths. The axial positions along the ingot of the slices on which IR measurements were made are shown in Figure 21(a). The radial measurement

<table>
<thead>
<tr>
<th>Sample number</th>
<th>Distance from tip (cm)</th>
<th>Mass density (g/cm²)</th>
<th>Average composition (x₁)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L6A8</td>
<td>0.80</td>
<td>7.1005</td>
<td>0.442</td>
</tr>
<tr>
<td>L6A10</td>
<td>1.00</td>
<td>7.1196</td>
<td>0.433</td>
</tr>
<tr>
<td>L6A12</td>
<td>1.20</td>
<td>7.2979</td>
<td>0.353</td>
</tr>
<tr>
<td>L6A17</td>
<td>1.65</td>
<td>7.5192</td>
<td>0.254</td>
</tr>
<tr>
<td>L6A20</td>
<td>2.00</td>
<td>7.5606</td>
<td>0.235</td>
</tr>
<tr>
<td>L6A24</td>
<td>2.40</td>
<td>7.5843</td>
<td>0.224</td>
</tr>
<tr>
<td>L6B135</td>
<td>3.50</td>
<td>7.6069</td>
<td>0.214</td>
</tr>
<tr>
<td>L6B148</td>
<td>4.85</td>
<td>7.6221</td>
<td>0.207</td>
</tr>
<tr>
<td>L6B162</td>
<td>6.25</td>
<td>7.6239</td>
<td>0.206</td>
</tr>
<tr>
<td>L6C2</td>
<td>7.75</td>
<td>7.6067</td>
<td>0.214</td>
</tr>
<tr>
<td>L6C5</td>
<td>9.25</td>
<td>7.6158</td>
<td>0.210</td>
</tr>
<tr>
<td>L6C7</td>
<td>10.25</td>
<td>7.6278</td>
<td>0.205</td>
</tr>
<tr>
<td>L6DT122</td>
<td>12.25</td>
<td>7.6247</td>
<td>0.206</td>
</tr>
<tr>
<td>L6ET119</td>
<td>13.80</td>
<td>7.6249</td>
<td>0.206</td>
</tr>
<tr>
<td>L6ET147</td>
<td>14.75</td>
<td>7.6428</td>
<td>0.138</td>
</tr>
<tr>
<td>L6ET157</td>
<td>15.75</td>
<td>7.6802</td>
<td>0.181</td>
</tr>
<tr>
<td>L6ET162</td>
<td>16.20</td>
<td>7.7101</td>
<td>0.168</td>
</tr>
<tr>
<td>L6FT169</td>
<td>16.90</td>
<td>7.8825</td>
<td>0.085</td>
</tr>
<tr>
<td>L6FT172</td>
<td>17.20</td>
<td>7.9895</td>
<td>0.082</td>
</tr>
<tr>
<td>L6FT177</td>
<td>17.70</td>
<td>8.0522</td>
<td>0.013</td>
</tr>
</tbody>
</table>
positions are shown in Figure 21(b). The diameter of the circles and their positions correspond to the width and relative locations of the incident infrared beam. Typical transmission data for slice A26 are shown in Figure 22. For slices A16, A26, E3, E39, and E34, the radial variation of the cut-on wavelengths and the corresponding alloy compositions are shown in Figure 23. Figure 24 shows the radial variation of the wavelength at 50% transmission. The radial compositional profiles indicate concave solid/liquid interfaces for the entire growth length and thus significant radial temperature gradients in the vicinity of the interface.

Figure 21. (a) Location of wafers along the growth axis of ingot L6 and (b) the IR measurement positions for a wafer.
Figure 22. Typical transmission spectra for a wafer (A26) from ingot L6. Numbers of curves refer to locations on wafer as shown in Figure 21.

Figure 23. Radial variations of the cut-on wavelength and Cd composition for ingot L6. Left-side plots are for areas 1 through 9 and right-side plots are for areas 10-13, 14-17 as shown in Figure 21.
4.5 Alloy Compositional Variation Along the Growth Axis

4.5.1 Theoretical Modeling

During directional solidification under conditions of complete mixing and near-equilibrium growth, the compositional variation along the growth axis is given by

\[ C_s(\xi) = k \, C_0 \, (1 - \xi)^{k-1}, \]  

(47)

where \( C_s(\xi) \) is the solute (CdTe) concentration at a distance \( \xi \) along an ingot of length \( L \), \( C_0 \) is the initial solute concentration in the melt, and \( k \) is the equilibrium distribution coefficient at the liquid-solid interface temperature. The distribution coefficient is given by \( k = x^S/x \), where \( x^S \) and \( x^L \) are respectively the solute compositions of the solid and the liquid at the interface temperature. In the derivation of Equation (47), \( k \) is assumed to be independent of the interface temperature.
Under conditions of elemental diffusion in the melt and negligible mixing, the compositional variation along the growth axis is dependent on the relative values of the interface translation rate, $R$, and the solute diffusion rate, $D$, in the melt. For $k > 1$ ($k < 1$), the solute distribution profile is expected to exhibit an initial transient of progressively decreasing (increasing) solute concentration, a region of constant composition equal to the original melt composition, and finally a region of rapidly decreasing (increasing) solute concentration. Smith, Tiller, and Rutter have examined the mathematical details of the problem and obtained analytical solutions for the transient compositional variations in terms of the material and growth parameters. Their solution for the initial composition-transient for constant $R$ and $k = 1$ given by

$$
\frac{C_s(t)}{C_0} = 1 + \text{erf} \left( \frac{1}{2} \left( \frac{R_l}{D} \right)^{1/2} \right) + (2k - 1)e^{-k(1-k)} \left( \frac{R_l}{D} \right)
$$

$$
\times \text{erfc} \left( \frac{2k - 1}{2} \right) \left( \frac{R_l}{D} \right)^{1/2}
$$

\begin{equation}
\tag{48}
\end{equation}

For the final composition-transient, they obtained the expression

$$
\frac{C_s(t)}{C_0} = 1 + \sum_{n=1}^{\infty} \frac{(2n + 1)}{n} \frac{(1 - k)(1 - k) \cdots (1 - k)}{(1 + k)(1 + k) \cdots (1 + k)} \frac{(n - k)}{(n + k)}
$$

\begin{equation}
\tag{49}
\times e^{-n(n+1)} \left[ R(L - t)/D \right]
\end{equation}

In the limit $R_l \gg D$, the widths of the initial and final transients are small, and $C_s(t)$ is essentially independent of $t$ and equal to $C_0$. For $R_l \gg D$ and $k > 0$, the axial compositional profile has an initial transient such that the first-to-freeze solid has a composition $C_s(0) = kC_0$, and with increasing $t$ the composition decreases to a steady-state value of $C_s(t) = C_0$. A final transient of rapidly decreasing composition occurs as the melt is consumed. The length of the central steady-state region can be increased at
prior to growth initiation and the uncertainties introduced by the tapered
gometry of the ampule tips, renders the initial-transient data unsuitable for
quantitative evaluations.

Figure 25. The variation of the interface segregation coefficient and interface translation
rate along the growth axis of ingot L3.
Figure 26. The variation of the interface segregation coefficient and interface translation rate along the growth axis of ingot L4.
Figure 27. The variation of the interface segregation coefficient and interface translation rate along the growth axis of ingot L6.
Figure 28. A comparison between the measured and calculated compositional profiles for ingot L3. The calculations assumed a diffusion coefficient of $6.0 \times 10^{-5}$ cm$^2$/s and included the variations in $k$ and $R$ along the growth axis.
Figure 29. A comparison between the measured and calculated compositional profiles for ingot L4. The calculations assumed a diffusion coefficient of $6.0 \times 10^{-5}$ cm$^2$/s and included the variations in $k$ and $R$ along the growth axis.
Figure 30. A comparison between the measured and calculated compositional profiles for ingot L6. The calculations assumed a diffusion coefficient of $4.5 \times 10^{-5} \text{ cm}^2/\text{s}$ and included the variations in $k$ and $R$ along the growth axis.

**Ingot: L6**

$Hg_{1-x}Cd_xTe$

$x = 0.202$

$L = 18.1$

$R_0 = 0.31 \mu \text{m/s}$

$k_0 = 3.63$

Calculated for

$D = 4.5 \times 10^{-5} \text{ cm}^2/\text{s}$

and varying $k$, $R$

Measured
Figure 31. A comparison between the experimental data for ingot L3 and calculated results for various values of the diffusion coefficient.
Figure 32. A comparison between the experimental data for ingot L4 and calculated results for various values of the diffusion coefficient.
Calculated for $D = 8.0 \times 10^{-5}$ cm$^2$/s and varying $\kappa$.

Figure 33: A comparison between the experimental data for Ingot L6 and calculated results for various values of the diffusion coefficient.
Figure 34. A comparison between the experimental data for ingot L3 and calculated results for a diffusion coefficient of $6.0 \times 10^{-5} \text{ cm}^2/\text{s}$ and constant $k, R$. 

Ingot L3

$Hg_1-x\text{xCd}_{x}\text{Te}$

$x = 0.200$

$L = 17.3 \text{ cm}$

$R_o = 0.597 \mu \text{m/s}$

$k_o = 3.63$
Figure 36. A comparison between the experimental data for ingot L4 and the calculated results for a diffusion coefficient of $6.0 \times 10^{-5}$ cm$^2$/s and constant $k$, $R$. 
Figure 36. A comparison between the experimental data for ingot L6 and the calculated results for a diffusion coefficient of $4.5 \times 10^{-5} \text{ cm}^2/\text{s}$ and constant $k$, $R$. 

Ingot L6
Hg$_{1.4}$Cd$_{0.6}$Te
$x = 0.202$
$L = 18.1 \text{ cm}$
$R_D = 0.31 \mu\text{m/s}$
$k_O = 3.63$

Calculated for
$D = 4.5 \times 10^{-5}$
and constant $k$, $R$

Measured

Distance along ingot (cm)

CdTe fraction, $x$
5. THEORETICAL MODELING OF CHARGE-CARRIER CONCENTRATIONS AND ELECTRON MOBILITIES

Theoretical models and computer programs specific to $\text{Hg}_1-x\text{Cd}_x\text{Te}$ were developed for calculations of charge-carrier concentrations, Hall coefficients, Fermi energies, and electron mobilities as functions of $x$, temperature, and ionized-defect and neutral-defect concentrations. As in previous work on the HgCdSe alloy system, the Kane three-band model is used to describe the $\text{Hg}_1-x\text{Cd}_x\text{Te}$ band structure for the energy range of interest, i.e., the lowest-lying conduction band ($\Gamma_6$) and the two highest-lying valence bands ($\Gamma_8$). Higher-band corrections considered in Reference 9 are neglected because such corrections are estimated to be small for the positive band-gap alloys that are of primary concern in this study. The electron mobilities are calculated in terms of a microscopic theory of electrical conduction derived from the solution of the Boltzmann equation for the perturbed steady-state electron distribution function.

5.1 Energy-Band Structure and Band Parameters

The secular equation describing the conduction, light-hole, and split-off-valence bands is

\[ E^3 + (\Delta - E_g) E^2 - (E \Delta + P^2 k^2) E - \frac{2}{3} \Delta P^2 k^2 = 0, \tag{54} \]

where $E$ is the band energy in terms of the crystal momentum wave vector $\hat{k}$, $\Delta$ is the $\Gamma_{15}$ spin-orbit splitting, $E_g$ is the $\Gamma_6 - \Gamma_8$ energy band-gap, and $P$ is the momentum matrix element between the $\Gamma_{15}$ valence-band and the $\Gamma_1$ conduction-band wave functions defined by Kane. The energies are referred to the top of the valence bands. The conduction, $c$, band and the light-hole, $lh$, band densities of states are given by

\[ p_i(E) = \frac{k^2}{\pi^2} \frac{dk}{dE} = \frac{1}{2\pi^2} \left( \frac{3}{\pi} \right)^{3/2} \frac{E^2}{P^3} \lambda_i \quad (i = c, lh), \tag{55} \]
where

\[ \lambda_c(\xi) = \frac{3[2\delta^2 \xi + \delta (3 - \delta) \xi^2 + \frac{4}{3} (1 - \delta) \xi - \frac{2}{3}] \left[ \xi(\xi - 1)(\delta \xi + 1) \right]^{1/2}}{2\left(\frac{3}{2} \delta \xi + 1\right)^{5/2}}, \]  

(56)

\[ \lambda_{d,h}(\xi) = \frac{3[2\delta^2 \xi^3 - \delta (3 - \delta) \xi^2 + \frac{4}{3} (1 - \delta) \xi + \frac{2}{3}] \left[ \xi(\xi + 1)(\delta \xi - 1) \right]^{1/2}}{2\left(\frac{3}{2} \delta \xi - 1\right)^{5/2}}, \]  

(57)

\[ \xi = E/E_g, \]  

(58)

and

\[ \delta = E_g/\Delta. \]  

(59)

The crystal momentum as a function of energy is

\[ k = \left(\frac{3}{2}\right)^{1/2} \frac{E_g}{\hbar} s(\xi), \]  

(60)

where

\[ s(\xi) = \left[ \frac{\xi(\xi - 1)(\delta \xi + 1)}{\left(\frac{3}{2} \delta \xi + 1\right)} \right]^{1/2}. \]  

(61)

The conduction-band wave functions are given by

\[ |\hat{k}, c, \pm\rangle = e^{i\hat{k}\cdot\hat{r}} \left[ a_\uparrow |1s\rangle \pm b|X \mp iY\rangle a_\downarrow \pm c|2\rangle a_\downarrow \right], \]  

(62)
where \( x, y, \) and \( z \) are the basis set of \( \Gamma_{15} \) referred to a coordinate system with the \( x \)-axis along \( \hat{r} \), \( S \) is the \( \Gamma_1 \) wave function, \( \sigma_{\pm} \) are Pauli spin functions for spin parallel (+) and anti-parallel (-) to \( \hat{r} \), and \( a, b, \) and \( c \) are functions defined by

\[
a = \left[ (\xi(\delta \xi + 1))^{1/2} \right] /
\]

\[
b = \sqrt{2} (\xi - 1)^{1/2} / 3N
\]

and

\[
c = (\xi - 1)^{1/2} (\delta \xi + \frac{2}{3}) / N,
\]

where

\[
N = \left[ (\xi(\delta \xi + 1))^{1/2} \right] /
\]

The heavy-hole, \( hh \), band is represented by a simple parabolic band given by

\[
E_{hh} = \frac{\hbar^2 k^2}{2m_e^* v_V^2},
\]

where \( v_V \) is the effective-mass ratio.

5.2 Calculation of the Temperature Dependence of the Carrier Concentrations

The Fermi energy, \( E_F \), electron concentration, \( n_e \), light-hole concentration, \( n_{lh} \), and the heavy-hole concentration, \( n_{hh} \), are calculated from the numerical solution of the charge neutrality equation,

\[
n_e - n_{lh} - n_{hh} = N_D - N_A,
\]

where
In Equation \( (71) \), \( F_{1/2}(-z) \) is the Fermi function of order \( 1/2 \), \( N_A \) and \( N_D \) are respectively the number of acceptors and donors per unit volume, \( k_B \) is the Boltzmann constant, \( T \) is the absolute temperature, \( m_o \) is the free electron mass, and \( y = E/k_B T \).

A literature search was performed to compile the best available band parameter values, and these band parameters along with the various material parameters required for the mobility calculations are summarized in Table 15. Using the values for the band parameters given in Table 15, the temperature and \( x \) dependences of the Fermi energies and carrier concentrations from 4.2 K to 300 K were calculated from Equations (67)-(70) for various net donor concentrations. The calculated results agree well with available data. A typical comparison between calculated and measured electron concentrations is shown in Figure 37 for an alloy composition of \( x = 0.183 \) and a net donor density \( N_D - N_A = 5.6 \times 10^{14} \text{ cm}^{-3} \).
Figure 37. Theoretical and experimental conduction-electron concentration for Hg$_{0.817}$Cd$_{0.183}$Te.

The graph shows the electron concentration ($n_e$) as a function of temperature (K). The theoretical and experimental curves are plotted, with the difference $N_D - N_A = 5.6 \times 10^{14}$ cm$^{-3}$ indicated.
### TABLE 15. PARAMETERS FOR ELECTRON-MOBILITY AND CHARGE-CARRIER-CONCENTRATION CALCULATION FOR Hg$_{1-x}$Cd$_x$Te ALLOYS.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spin-orbit splitting$^{(a)}$</td>
<td>$\Delta_0 = (-0.18x + 1.08)$ eV</td>
<td>(1)</td>
</tr>
<tr>
<td>Heavy-hole mass$^{(b)}$</td>
<td>$m_{hh}/m_0 = 0.53$</td>
<td>(2)</td>
</tr>
<tr>
<td>Deformation potentials$^{(c)}$</td>
<td></td>
<td>(3)</td>
</tr>
<tr>
<td>Longitudinal sound velocity$^{(d)}$</td>
<td>$v_L = (2.52 + 0.54x) \times 10^5$ cm/s</td>
<td></td>
</tr>
<tr>
<td>Transverse sound velocity$^{(d)}$</td>
<td>$v_T = (1.60 + 0.27x) \times 10^5$ cm/s</td>
<td></td>
</tr>
<tr>
<td>Hg mass</td>
<td>$m_{Hg} = 200.59$ a.m.u.</td>
<td></td>
</tr>
<tr>
<td>Cd mass</td>
<td>$m_{Cd} = 112.4$ a.m.u.</td>
<td></td>
</tr>
<tr>
<td>Te mass</td>
<td>$m_{Te} = 127.60$ a.m.u.</td>
<td></td>
</tr>
<tr>
<td>Lattice constant</td>
<td>$a_0 = (0.6460 + 0.0021x) \text{ nm}$</td>
<td>(5)</td>
</tr>
<tr>
<td>$\Gamma_6$-$\Gamma_8$ energy gap</td>
<td>$E_g = [-0.03 + 5 \times 10^{-4} x + (1.91 - 10^{-3} x) x] \text{ eV}$</td>
<td>(6)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E_g = [-0.303 + 1.73x + 5.6 \times 10^{-4} (1 - 2x) T$</td>
<td>(7)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$+ 0.25x^2] \text{ eV (0.23} \leq x \leq 0.61, 10 K \leq T \leq 300 \text{ K)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$E_g = [-0.25 x 1.59 x + 5.233 \times 10^{-4} (1 - 2.08x) T$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$+ 0.327x^2] \text{ eV (0.13} \leq x \leq 0.6, 20 K \leq T \leq 300 \text{ K)}$</td>
</tr>
<tr>
<td>Momentum matrix element coupling conduction and valence bands$^{(e)}$</td>
<td>$P = 8.55x \times 10^{-8}$ eV$\cdot$cm</td>
<td></td>
</tr>
<tr>
<td>Transverse effective charges</td>
<td>HgTe: $e_T/e^* = 2.96$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CdTe: $e_T/e^* = 2.35$</td>
<td></td>
</tr>
<tr>
<td>Reduced masses</td>
<td>$m_{HgTe} = 1.295 \times 10^{-22} \text{ g}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$m_{CdTe} = 9.923 \times 10^{-23} \text{ g}$</td>
<td></td>
</tr>
<tr>
<td>Dielectric constants$^{(f)}$</td>
<td>$\varepsilon_0 = 20.206 - 15.153x + 6.59091x^2$</td>
<td>(9)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$-0.951826x^3$</td>
</tr>
<tr>
<td></td>
<td>$\varepsilon_{\infty} = 15.1077 - 13.8823x + 9.88928x^2$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$- 3.67133x^3$</td>
</tr>
<tr>
<td>HgTe LO phonon frequency</td>
<td>$\omega_{HgTe}^{LO} = (139 - 9x) \text{ cm}^{-1}$</td>
<td></td>
</tr>
<tr>
<td>HgTe TO phonon frequency</td>
<td>$\omega_{HgTe}^{TO} = (118 + 12x) \text{ cm}^{-1}$</td>
<td></td>
</tr>
<tr>
<td>CdTe LO phonon frequency</td>
<td>$\omega_{CdTe}^{LO} = (154 + 16x) \text{ cm}^{-1}$</td>
<td>(9)</td>
</tr>
<tr>
<td>CdTe TO phonon frequency</td>
<td>$\omega_{CdTe}^{TO} = (152 - 9x) \text{ cm}^{-1}$</td>
<td></td>
</tr>
</tbody>
</table>

---

*ORIGINAL PAGE IS OF POOR QUALITY*
(a) $\Delta_0 - \Gamma_8 - \Gamma_7$ at $k = 0$. A linear interpolation was made between the HgTe value and the CdTe value.

(b) $x = 0$, zone center

(c) The $E_1$ value is for CdTe (i.e., $x = 1$). The variation of $E_1$ with $x$ has not been considered. The value of $E_2$ is estimated based on a hydrogenic approximation.

(d) $V_\perp^2 = c_{11}/\rho$, $V_\parallel^2 = c_{44}/\rho$, $\rho = \left(\frac{1}{2.34} \times 8\right) \text{ g/cm}^3$ [This approximate equation was obtained using data from J. Blair and R. Newnham (10)]. The value of $c_{11}$ for HgTe (300 K) is 50.8 GPa (11), while the value for CdTe is 53.5 GPa (12, 13). The assumption of a linear variation for $c_{11}$ as a function of $x$ yields the result. $c_{11} = (2.7x + 50.8) \text{ GPa}$. The value of $c_{44}$ for HgTe (300 K) is 70.5 GPa (12), while the value for CdTe is 19.9 GPa (12). Assuming a linear variation for $c_{44}$ as a function of $x$, $c_{44} = \left((-0.60x + 20.5) \text{ GPa}\right)$. These values for $\rho$, $c_{11}$, and $c_{44}$ yield the composition dependence for the velocities given in the table.

(e) The value of $P$ was calculated from the equation $\hbar^2/m_0^* = (2\hbar^2/3) \left[2/E_g + 1/(E_g + \Delta)\right]$, where $x = 0.204$ and values of $m_0^* = 4.66 \times 10^{-3} m_0$, $E_g = 51.7 \times 10^{-3} \text{ eV}$, and $\Delta = 0.06 \text{ eV}$ were used (14).

(f) These approximate equations were obtained using the referenced data.


---

1 A good compilation of data on the properties of Hg$_{1-x}$Cd$_x$Te is given by R. Dornhaus and G. Nintz, Springer Tracts in Modern Physics, Solid State Physics, (Springer-Verlag, 1976) Vol. 78, p. 1 ff.
5.3 Theoretical Modeling of the Electron Mobility

The electron mobility calculation includes the following scattering mechanisms: longitudinal-optical phonon (LO), longitudinal- and transverse-acoustical phonon (ac), heavy-hole (hh), and alloy disorder potential (dis.). The extrinsic scattering mechanisms include charged (ii) and neutral point-defects (nd). The current densities, conductivities, and mobilities are calculated from the perturbed electron distribution function $f(k)$ given by

$$f(k) = f_o - kc'(E) f_o' \cos \psi,$$

where $f_o$ is the unperturbed distribution function and $f_o' = \frac{df}{dE}$. The quantity $\psi$ is the angle between the wavevector $k$ and the applied electric field. The perturbation function $c'(E)$ depends only on the energy. The current density is given by

$$J = e \frac{1}{3 \pi^2 \hbar} \int_{E_g}^{\infty} k^2 c'(E) f_o' dE,$$

where $e$ is the electronic charge, $\hbar$ is Planck's constant, and $c'(E)$ is given by the solution of the Boltzmann equation,

$$\frac{\partial f(k)}{\partial t} = \sum_i \left( \frac{\partial f}{\partial t}_i \right) + \left( \frac{\partial f}{\partial t} \right)_F (i = \text{LO, ac, eh, dis., ii, nd}).$$

The sum, $\sum_i \left( \frac{\partial f}{\partial t}_i \right)$, is the rate of change of the distribution function caused by the various scattering mechanisms, and $\left( \frac{\partial f}{\partial t} \right)_F$ is the rate of change of the distribution function caused by the application of a static electric field. For the steady-state,

$$\frac{\partial f(k)}{\partial t} = 0.$$
and
\[ \sum_{i} \frac{\partial f_i}{\partial t} = - \frac{\partial f_i}{\partial t} \text{.} \]

The field term is given by
\[ \left( \frac{\partial f}{\partial t} \right)_F = \frac{\varepsilon E_0}{\hbar} f_o \cos \psi, \]
where \( \varepsilon \) is the applied electric field. The scattering term is given by\(^{28}\)
\[ \sum_{i} \frac{\partial f_i}{\partial t} = - \frac{1}{k_B T} \sum_{k} \int V_1 (k, k') \left[ k c'(E') - k' c'(E) \right] dk' \cos \psi, \]
where
\[ V_1 (k, k') = W_1 (k', k) f_o (k') \left[ 1 - f_o (k) \right] = V_1 (k', k). \]

\( W_1 (k', k) \) is the transition probability per unit time per unit volume and is given by
\[ W_1 (k', k) = \left| H_1 (k', k) \right|^2 \left( \frac{1}{3 \hbar^2} \right) \Omega \left( E_{k'} - E_{k} \pm E_S \right), \]
where \( H_1 (k', k) \) is the matrix element for scattering from state \( k \) to \( k' \) for a given scattering process, \( \Omega \) is a delta function, and \( E_S \) is the energy absorbed or emitted in the scattering process.

Equation (79) reduces to a linear finite-difference equation in \( c'(E) \), and the conductivity is determined from Equation (76) by using the variational method of Kohler\(^{28}\) as modified by Howarth and Sondheimer\(^{27}\) and Ehrenreich\(^{29}\). The perturbation function is expanded in a complete set of trial functions,
\[ c'(E) = \sum_{n=0}^{\infty} c_n \phi_n (E), \]
and the $c_n$ are determined by the requirement that $c'(E)$ be a stationary point\textsuperscript{28} of a certain conserved integral.

The various scattering mechanisms and their contributions to the Boltzmann equation are summarized in Appendix A. The computer program for calculating the Fermi energy, the charge-carrier concentrations, and the electron mobilities is given in Appendix B.

5.4 Calculations of the Temperature Dependence of the Electron Mobility

Calculations were performed to ascertain the relative contributions of the various scattering mechanisms to the conduction electron mobility as functions of temperature from 4.2 K to 300 K for alloy compositions near $x = 0.2$. The material parameters used in the calculations are given in Table 15. Figures 38 and 39 show the calculated results for the sample described in Figure 37. The curves designated by the symbols $\mu_{LO}$, $\mu_{ac}$, $\mu_{dis}$, $\mu_{eh}$ and $\mu_{ii}$ correspond to the calculated mobilities for the individual scattering mechanisms. The calculations shown in Figure 38 were made assuming that all ionized defects are donors, i.e., the donor density is equal to the residual conduction-electron density at low temperatures ($T \lesssim 50$ K). The calculated results in Figure 39 assumed a donor density of $N_D = 7.6 \times 10^{14} \text{ cm}^{-3}$ and an acceptor density of $2.0 \times 10^{14} \text{ cm}^{-3}$. The calculated results indicate that for alloy compositions of $x = 0.2$, longitudinal optical-phonon scattering is the dominant mobility-limiting mechanism at high temperatures ($\gtrsim 75$ K), while ionized-defect scattering is the dominant mechanism at low temperatures ($\lesssim 75$ K).

The agreement between the temperature dependence of the calculated total mobility, $\mu_T$, and the experimental data is reasonably good. However, as the temperature increases, the calculated and measured mobilities systematically diverge until at 300 K the calculated mobilities are about a factor of two higher than experimental values. A probable reason for this discrepancy is an overestimate of the screening of the electron-LO-phonon interaction. The approximate screening function used in the calculations treats the electrons as always screening and ignores the possible antiscreening effects considered by Ehrenreich\textsuperscript{30} for small momentum transfers. The calculations also neglect possible scatterings by neutral point-defects and by line-defects. These,
combined with the uncertainties in the various material parameters, could explain the differences between the calculated and measured results.

Figure 38. A comparison of the temperature dependence of the calculated and measured conduction-electron mobilities for an alloy composition of $x = 0.183$. The calculated results are for a donor concentration equal to the residual electron concentration in Figure 37.
Figure 39. A comparison of the temperature dependence of the calculated and measured conduction-electron mobilities for an alloy composition of $x = 0.183$. The calculations assumed a donor concentration of $7.6 \times 10^{14}$ cm$^{-3}$ and an acceptor concentration of $2 \times 10^{14}$ cm$^{-3}$. 

Donor density = $7.6 \times 10^{14}$ cm$^{-3}$

Acceptor density = $2 \times 10^{14}$ cm$^{-3}$

Disorder energy = 2 eV
REFERENCES


APPENDIX A: ELECTRON SCATTERING MECHANISMS AND THE SOLUTION TO THE BOLTZMANN EQUATION.

The mathematical expressions used for the various scattering mechanisms are essentially the same as those used for the calculations of electron mobilities in the HgCdSe alloys described in References 9 and 10. Some of the pertinent mathematical details are included as part of this report to aid in interpretation of the computer programs.

A.1 Longitudinal-Optical (LO) Phonon Scattering Mechanism

The strength of the LO-phonon/electron interaction is proportional to the Callen effective charge, \( e_\text{c}^* \), associated with relative displacements of atoms in a unit cell. The Callen effective charge is related to the Szigeti effective charge, \( e_\text{s}^* \), and the total transverse charge, \( e_\text{T}^* \), by the relations

\[
\frac{e_\text{c}^*}{e_\text{s}^*} = \left[ \frac{\varepsilon_\infty + 2}{3 \varepsilon_\infty} \right] e_\text{s}^* \quad (A1)
\]

and

\[
\frac{e_\text{s}^*}{e_\text{T}^*} = \frac{e_\text{T}^*}{e_\infty} \quad (A2)
\]

where \( \varepsilon_\infty \) is the high-frequency dielectric constant. The interaction is assumed to be screened by the dielectric function given by

\[
\varepsilon(\omega_L, q) = \varepsilon_\infty + \frac{(k_{\text{FT}}^e)^2 + (k_{\text{FT}}^{\text{lh}})^2}{q^2} \quad (A3)
\]

where \( \omega_L \) is the longitudinal-phonon frequency, \( q \) is the phonon wave vector, and \( k_{\text{FT}}^e \) and \( k_{\text{FT}}^{\text{lh}} \) are the electron and light-hole Fermi-Thomas momenta given by
where

\[ \mu' = 3/2 \frac{E}{c^2 m_N^2} \]

and the other parameters have been defined in Sections 5.1 and 5.2.

The scattering term of the Boltzmann equation for the LO-phonon-electron interaction is given by

\[ \left( \frac{\partial f(k)}{\partial t} \right)_{LO} = - \frac{e^2 \mu' \omega_{LO} k_B T (F_1 + F_2)}{\hbar \omega_{LO} \beta} \mathcal{L}\left( c' \right) f' \cos \psi, \]  

(A7)

where

\[ F_i = \frac{4 \pi N_i e_{T_i}^2}{M_i} \quad (i = 1 = \text{HgTe}, i = 2 = \text{CdTe}), \]  

(A8)

\( N_i \) is the number of unit cells of the \( i \)th type per unit volume, \( M_i \) is the reduced mass of the \( i \)th unit cell, and

\[ \mathcal{L}\left( c' \right)_{LO} = 1 \left\{ \frac{f_+ / f_0}{(n_p + 1) (c'_+ R'_+ - c'_+ S'_+)} + \frac{f_- / f_0}{n_p (c'_- R'_- - c'_- S'_-)} \right\}. \]  

(A9)

The subscripts \((\pm)\) refer to the evaluation of the function at \( y \pm \theta \), where
\[ y = E/k_B T \text{ and } \theta = \hbar \omega_k / k_B T. \]

The function, \( n_p \), is the phonon occupation number given by

\[ n_p = (e^\theta - 1)^{-1}. \]  \hspace{1cm} (A10)

The functions \( R_\pm \) and \( S_\pm \) are defined as follows:

\[ R_\pm(y, \theta) = F_\lambda(y)F_\lambda(y \pm \theta)(s_{\pm}^2 + s^2) \sum_{n=0}^{2} \rho_n^\pm(y, \theta) v_{n+1}^\pm(y, \theta) , \]  \hspace{1cm} (A11)

\[ S_\pm(y, \theta) = F_\lambda(y)F_\lambda(y \pm \theta) s^2(s_{\pm}^2 + s^2) \sum_{n=0}^{2} \rho_n^\pm(y, \theta) v_n^\pm(y, \theta) , \]  \hspace{1cm} (A12)

\[ F_\lambda(y) = \frac{2 2 y^3 + 3 \delta (3 - \delta) y^2 + \frac{4}{3} (1 - \delta) y - \frac{2}{3}}{\sqrt{\frac{2}{3} \delta y + 1}^2} , \]  \hspace{1cm} (A13)

\[ b_1 = \left( \frac{\sqrt{2}}{3N(\delta y)} \right) \left( \frac{\sqrt{2}}{3} \delta y + 1 \right) \frac{1}{\delta y(\delta y + 1)} \right) \right)^{1/2}, \]  \hspace{1cm} (A14)

\[ c_1 = \left( \frac{\delta y + \frac{2}{3}}{N(\delta y)} \right) \left( \frac{\sqrt{2}}{3} \delta y + 1 \right) \frac{1}{\delta y(\delta y + 1)} \right) \right)^{1/2}, \]  \hspace{1cm} (A15)

\[ \rho_0^\pm(y, \theta) = (aa_\pm)^2 - bb_\pm(ba_\pm + cb_\pm)/\sqrt{2} \]  \hspace{1cm} (A16)

\[ + \frac{1}{2} (bc_\pm + cb_\pm)^2 + \frac{1}{4} (bb_\pm)^2 , \]

\[ \rho_1^\pm(y, \theta) = 2aa_\pm(b_1b_1^\pm + c_1c_1^\pm) , \]  \hspace{1cm} (A17)
\[ \rho_2^\pm (y, \theta) = \frac{3}{4} \left( b_1 b_{1\pm} \right)^2 + b_{1\pm} b_{1\pm} \left( (b_1 c_{1\pm} + c_1 b_{1\pm}) / \sqrt{2} \right) \]

\[ + 2 b_{1\pm} c_{1\pm} b_{1\pm} - \frac{1}{2} (b_1 c_{1\pm} + c_1 b_{1\pm})^2 + (c_1 c_{1\pm})^2, \]

(A18)

\[ v_0^\pm (y, \theta) = -\frac{1}{q_\pm} \left( \frac{2 p_\pm^2}{p_\pm^2 - 4 r_\pm^2} + \frac{1}{2} \ln \left| \frac{p_\pm - 2 r_\pm}{p_\pm + 2 r_\pm} \right| \right), \]

(A19)

\[ v_1^\pm (y, \theta) = r_\pm \left( \frac{p_\pm}{p_\pm^2 - 4 r_\pm^2} - \frac{1}{q_\pm} - \frac{p_\pm^2}{q_\pm (p_\pm^2 - 4 r_\pm^2)} \right) \]

(A20)

\[ + \frac{1}{4} \left( 1 - \frac{2 p_\pm}{q_\pm} \right) \ln \left| \frac{p_\pm - 2 r_\pm}{p_\pm + 2 r_\pm} \right|, \]

\[ v_2^\pm (y, \theta) = \frac{1}{4} \left( r_\pm \left[ 1 - \frac{2 p_\pm}{q_\pm} + \left( 1 - \frac{p_\pm^2}{q_\pm} \right) \frac{r_\pm^2}{p_\pm^2 - 4 r_\pm^2} \right] \right) \]

(A21)

\[ + \frac{p_\pm}{2} \left( 2 - \frac{3 p_\pm}{q_\pm} \right) \ln \left| \frac{p_\pm - 2 r_\pm}{p_\pm + 2 r_\pm} \right|, \]

\[ v_3^\pm (y, \theta) = -\frac{r_\pm^3}{3 q_\pm} + \frac{p_\pm r_\pm}{2} \left( 1 - \frac{3 p_\pm}{2 q_\pm} + \frac{p_\pm^2}{2 (p_\pm^2 - 4 r_\pm^2)} \right. \]

\[ - \frac{p_\pm^3}{2 q_\pm (p_\pm^2 - 4 r_\pm^2)} + \frac{p_\pm^2}{16} \left( 3 - \frac{4 p_\pm}{q_\pm} \right) \ln \left| \frac{p_\pm - 2 r_\pm}{p_\pm + 2 r_\pm} \right|, \]

(A22)

\[ q_\pm = s_\pm^2 + s^2, \]

(A23)
\[ p_\pm = q_\pm + \varepsilon_\omega^2, \quad (A24) \]

\[ r_\pm = \varepsilon_\omega^2, \quad (A25) \]

and

\[ \varepsilon_\omega^2 = \frac{n^2}{2\nu m_0 E_\omega} \left[ \left( k_{FT}^e \right)^2 + \left( k_{FT}^h \right)^2 \right]. \quad (A26) \]

The symbols \( a, b, \) and \( c \) have been defined in Section 5.1. In the above, \( R_- \) and \( S_- \) are zero for \( y - \theta - \beta^{-1} < 0. \)

\subsection*{A.2 Acoustical Phonon (ac) Scattering Mechanism}

The longitudinal and transverse acoustical-phonon/electron interactions are characterized by three deformation potentials: \( k_0 \) for the longitudinal mode and \( E_1 \) and \( E_2 \) for the transverse modes. The acoustical-phonon contribution to the Boltzmann equation is given by

\[ \left( \frac{3\varepsilon(k)}{\delta t} \right)_{ac} = \frac{2k^T E_0^2}{5 \hbar \rho_m v_L} \left( \nu_{m_0} \right)^2 E_\omega \lambda_c \]

\[ \times \left[ F_L + \left( \frac{v_L}{v_T} \right)^2 F_T \right] f_0 \cos \psi \cos \psi(E), \quad \text{(A27)} \]

where \( \rho_m \) is the mass density of the material, and \( v_L \) and \( v_T \) are the longitudinal and transverse velocities of sound, respectively.

The longitudinal and transverse scattering functions, \( F_L \) and \( F_T \), are given by

\[ F_L = A_1^2 + \frac{2}{3} (A_1 A_2 + A_4) + \frac{1}{2} (2A_1 A_3 + A_2^2 - A_4) \]

\[ + \frac{4}{5} A_2 A_3 + \frac{1}{3} A_3^2 \quad \text{(A28)} \]
\[ F_T = \left( \frac{E_1}{E_0} \right)^2 \left( B_1 + \frac{2}{3} B_2 + \frac{1}{2} B_3 + \frac{2}{5} B_4 + \frac{1}{3} B_5 + B_6 \right), \tag{A29} \]

where

\[ A_1 = a^2 + \left( \frac{E_1}{E_0} \right)^2 \left( \frac{1}{2} b^2 \right) + \left( \frac{E_2}{E_0} \right) \left( c^2 + \frac{1}{2} b^2 \right), \tag{A30} \]

\[ A_2 = -\left( \frac{E_1}{E_0} \right) \left( c^2 + \frac{1}{2} b^2 \right) + \left( \frac{E_2}{E_0} \right) \left( 5c^2 + \frac{1}{2} b^2 \right), \tag{A31} \]

\[ A_3 = 4\left( \frac{E_2}{E_0} \right) \left( c^2 - \frac{1}{2} b^2 \right), \tag{A32} \]

\[ A_4 = \left( \frac{E_1}{E_0} \right)^2 b^2 c^2, \tag{A33} \]

\[ B_1 = \frac{1}{4} b^4, \tag{A34} \]

\[ B_2 = -b^2 \left[ b(b + \sqrt{2} c) + \frac{1}{4} b^2 - (b + c/\sqrt{2})^2 \right], \tag{A35} \]

\[ B_3 = b^2 \left[ (b + \sqrt{2} c)^2 + b(b + \sqrt{2} c) - 2(b + c/\sqrt{2})(b + \sqrt{2} c) \right. \]
\[ \left. \quad - (b + c/\sqrt{2})^2 \right], \tag{A36} \]

\[ B_4 = 2b^2 \left( b + c/\sqrt{2} \right) \left( b + \sqrt{2} c \right), \tag{A37} \]
\[ B_5 = -b^2(b + \sqrt{2}c)^2, \tag{A38} \]

and

\[ B_6 = \frac{1}{2} [b^2c^2 + \frac{1}{3}(c^2 - \frac{1}{2}b^2)^2]. \tag{A39} \]

A.3 Ionized Impurity (ii) Scattering Mechanism

The electron/ionized-defect interaction is assumed to be screened by the dielectric function

\[ \varepsilon(q) = \varepsilon_0 + \frac{1}{q} \left[ (k_{\text{FT}}^e)^2 + (k_{\text{FT}}^h)^2 + (k_{\text{FT}}^{\text{hh}})^2 \right], \tag{A40} \]

where \( k_{\text{FT}}^{\text{hh}} \) is the heavy-hole Fermi-Thomas momentum, given by

\[ (k_{\text{FT}}^{\text{hh}})^2 = \frac{2}{\pi} \left( \frac{2\mu_m \alpha}{\hbar^2} \right)^{3/2} (k_B T)^{1/2} F_{-1/2}(-z), \tag{A41} \]

\( \varepsilon_0 \) is the low-frequency dielectric constant, and \( F_{-1/2} \) is the Fermi function of order \(-1/2\).

The contribution to the Boltzmann equation from ionized-impurity scattering is

\[ \left( \frac{\partial f(k)}{\partial t} \right)_{\text{ii}} = \frac{\pi (N_D^2 + N_A Z_A^2) e^4 \lambda}{h^2 E s^3} \varepsilon_0 f_o \phi_{\text{ii}} \cos \psi c'(E), \tag{A42} \]

where \( N_D \) and \( N_A \) are the donor and acceptor concentrations, respectively, and \( Z_D \) and \( Z_A \) are their charges in electron-charge units. The scattering function, \( \phi_{\text{ii}} \), is given by
\[ \phi_{11} = \sum_{n=0}^{2} \pi_n \phi_n, \quad (A43) \]

where

\[ \phi_0 = \ln\left(\frac{\phi_0^2 + 4a^2}{\phi_0^2}\right) - \frac{4a^2}{\phi_0^2 + 4a^2}, \quad (A44) \]

\[ \phi_1 = \frac{\phi_0^2 + 4a^2}{2a^2} \ln \left(\frac{\phi_0^2 + 4a^2}{\phi_0^2}\right) - \frac{4(\phi_0^2 + 3a^2)}{(\phi_0^2 + 4a^2)}, \quad (A45) \]

\[ \phi_2 = \frac{\phi_0^2}{2a^2} \left[ -4\frac{(\phi_0^2 + s^2)}{\phi_0^2} + \frac{(\phi_0^2 + 2s^2)^2 + 4(\phi_0^2 + 2s^2)}{2s^2 \phi_0^2} \right] \]

\[ \times \ln \left(\frac{\phi_0^2 + 4a^2}{\phi_0^2}\right) - \frac{2(\phi_0^2 + 2s^2)^2}{\phi_0^2 (\phi_0^2 + 4a^2)}, \quad (A46) \]

\[ \pi_0 = a^4 + \frac{1}{4} b^4 - \sqrt{2} b^3 c + 2b^2 c^2, \quad (A47) \]

\[ \pi_1 = 2a^2 (b^2 + c^2), \quad (A48) \]

\[ \pi_2 = \frac{3}{4} b^4 + \sqrt{2} b^3 c + c^4, \quad (A49) \]
Electron-Hole (eh) Scattering Mechanism

The contribution to the Boltzmann equation from electron-hole scattering is

\[ \frac{\delta^2}{\delta t^2} \left( \frac{\partial f(k)}{\partial k} \right)_{eh} = \frac{\pi}{\hbar c} e^{\lambda} \left( \frac{\hbar^2}{m_e} \right)^2 \frac{f_{eh} c' \cos \psi c'(E)}{E_0} \]

where \( f_{eh} \) is the same as \( f_{II} \) for ionized defect scattering except that \( E_0 \) is replaced by \( E_m \), i.e.,

\[ \frac{\delta^2}{\delta t^2} \left( \frac{\partial f(k)}{\partial k} \right)_{eh} = \frac{\pi}{\hbar c} e^{\lambda} \left( \frac{\hbar^2}{m_e} \right)^2 \frac{f_{eh} c' \cos \psi c'(E)}{E_m} \]

A.4 Compositional-Disorder (dis.) Scattering Mechanism

Electron scattering by the random short-range potentials resulting from alloy compositional disorder is treated as scattering by a random distribution of square-well scattering centers, which have unit-cell dimensions and depths approximately equal to the difference in band gaps between CdTe and HgTe. The contribution to the Boltzmann equation from this process is given by

\[ \left( \frac{\delta^2 f(k)}{\delta t^2} \right)_{dis.} = \frac{E_{dis.}^2}{\hbar^2} \left( \frac{\mu m_e}{\hbar} \right)^2 \frac{x (1 - x) E_{dis.}^2}{N_a} \frac{\phi_{dis.} c' \cos \psi}{c_0} \]

where \( N_a \) is the number of unit cells per unit volume, \( E_{dis.} \) is the disorder potential, approximately equal to the difference in CdTe and HgTe band gaps, and \( \phi_{dis.} \) is a wave-function-overlap integral given by

\[ \phi_{dis.} = \int \phi_{\text{CdTe}}(r) \phi_{\text{HgTe}}(r) \]
A.6 Neutral-Defect (nd) Scattering Mechanism

The scattering of electrons by neutral point-defects is also described in terms of scattering by a random distribution of square-well potentials. Thus the contribution of neutral point-defects to the Boltzmann equation is also given by Equation (A53) with $x(1-x) E_{\text{dis.}}^2 / N_a$ replaced by $N_n n^{-2} E_{n}^2$, where $N_n$ is the density of neutral point-defects, $n_n$ is the volume of the potential well, and $E_{n}$ is the strength.

A.7 Calculation of the Electron Mobility

The total scattering contribution to the Boltzmann equation from the scattering mechanisms considered is

$$
\sum_{i=1}^{3} \left( \frac{\partial f(k)}{\partial t} \right)_i = - \frac{e^2}{\hbar^2} \sum_{i=1}^{3} \frac{m}{\lambda s} \frac{1}{E_{\text{eff}}} \left[ F_1 + F_2 \right] \mathcal{P}(c') f' \cos \psi,
$$

where

$$
\mathcal{P}(c') = \mathcal{P}(c') - \left\{ a_{ac} \lambda_c^2 s^2 \left[ F_L + \left( \frac{\gamma_L}{V_T} \right)^2 F_T \right] + a_{ii} \frac{\lambda^2_c}{s^2} \phi_{ii} \right. \\
+ a_{eh} \frac{c^2}{s^2} \phi_{eh} + (a_{\text{dis.}} + a_n) \lambda^2 c s^2 \phi_{\text{dis.}} \left\} c'(E),
$$

with the following defined quantities:
The substitution of Equation (A55) into the steady-state Boltzmann equation, Equation (79), yields the following linear finite-difference equation:

\[ \mathcal{L}(c') = \frac{2^{1/2} \sigma n^2 \omega_w e}{e (\mu m_0)^{3/2} (F_1 + F_2)} \left( k_B T \right)^{1/2} \frac{\sigma^2}{\beta^{3/2}}. \] (A62)

To obtain a solution, the perturbation function, \( c'(E) \), is expanded in a complete set of trial functions,

\[ c'(E) = \sum_{n=0}^{\infty} c_n \phi_n(E). \] (A63)
and the $c_n$ are determined by the requirement that $c'(E)$ be a stationary point of a certain conserved integral. The set,

$$
\phi_n = (y - \beta^{-1})^n, \quad (A64)
$$

is used for the trial functions, and the expansion is carried to third order (i.e., $n = 2$). The current density $J_x$, Equation (75), is given by

$$
J_x = \frac{4e^2 \omega L (k_B T)^2}{3 \pi^2 \hbar^2 (v_1 + F_2)} \left\{ F_{00} + \frac{[(L, L)_{1}]^2}{L_2 L_1} + \frac{[(L, L)_{2}]^2}{L_3 L_2} + \ldots \right\}, \quad (A65)
$$

where

$$
\mathcal{L}_{n+1} = \begin{bmatrix}
F_{00} & \cdots & F_{01} & \cdots & F_{0n} \\
F_{10} & & \ddots & & \vdots \\
\vdots & & \ddots & & \vdots \\
F_{n0} & \cdots & \cdots & \cdots & F_{nn}
\end{bmatrix}, \quad (A66)
$$

$$
(\mathcal{L}, \mathcal{L})_n = \begin{bmatrix}
F_{00} & \cdots & F_{0,n-1} & L^{(0)} \\
\vdots & & \ddots & \vdots \\
F_{n0} & \cdots & \cdots & L^{(n)}
\end{bmatrix}, \quad (A67)
$$

$$
F_{mn} = \int_{\beta^{-1}}^{\infty} \phi_m \mathcal{S}(\phi_n) \phi'_o \, dy, \quad (A68)
$$

and

$$
L^{(n)} = \int_{\beta^{-1}}^{\infty} \phi_n \phi'_o \frac{s^3}{\beta^{3/2}} \, dy. \quad (A69)
$$
The electrical conductivity, $\sigma$, is given by the relation

$$\sigma = J_x / \varepsilon,$$

and the electron mobility is given by

$$\mu = \sigma / n_e.$$
APPENDIX B: COMPUTER PROGRAMS FOR CALCULATION OF CHARGE CARRIER CONCENTRATIONS AND ELECTRON MOBILITIES

B.1 Description of Symbols - Main Program

<table>
<thead>
<tr>
<th>Line no.</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>00330</td>
<td>Input parameters: TMIN = minimum temperature (K), TMAX = maximum temperature (K), DELT = temperature increment, DONOR DENSITY (cm(^{-3})), ACCEPTOR DENSITY (cm(^{-3})), PROPORTION OF CdTe IN ALLOY (at.%), DISORDER ENERGY IN (eV).</td>
</tr>
<tr>
<td>00500</td>
<td>ES = electron charge in c.g.s. units.</td>
</tr>
<tr>
<td>00510</td>
<td>HB = Planck's constant (erg-s).</td>
</tr>
<tr>
<td>00520</td>
<td>K = Boltzmann's constant (erg/K).</td>
</tr>
<tr>
<td>00530</td>
<td>MO = free electron mass (g).</td>
</tr>
<tr>
<td>00540</td>
<td>PI = (\pi).</td>
</tr>
<tr>
<td>00550</td>
<td>CEVE = units conversion factor (eV to ergs).</td>
</tr>
<tr>
<td>00560</td>
<td>FFCTS is an external program for evaluating Fermi functions. A separate data file of the values of Fermi functions is required.</td>
</tr>
<tr>
<td>00705</td>
<td>X2 = at.% of CdTe in alloy, (x).</td>
</tr>
<tr>
<td>00706</td>
<td>X1 = at.% of HgTe in alloy, (1 - x).</td>
</tr>
<tr>
<td>00741</td>
<td>HCSPOL is an external program used for determining a number of parameters used in the calculations.</td>
</tr>
<tr>
<td>00790</td>
<td>TMIN = minimum temperature (K).</td>
</tr>
<tr>
<td>00800</td>
<td>TMAX = maximum temperature (K).</td>
</tr>
<tr>
<td>00810</td>
<td>DTEMP = temperature increment.</td>
</tr>
<tr>
<td>00820</td>
<td>ND = donor density.</td>
</tr>
<tr>
<td>00840</td>
<td>NA = acceptor density.</td>
</tr>
<tr>
<td>00880</td>
<td>DEV = spin-orbit splitting (in eV) as a function of (x).</td>
</tr>
<tr>
<td>00885</td>
<td>D = spin-orbit splitting (in ergs) as a function of (x).</td>
</tr>
<tr>
<td>00890</td>
<td>UV = heavy hole mass (in electron mass units)</td>
</tr>
<tr>
<td>00960 to</td>
<td>E0EV, E1EV, and E2EV are deformation potentials in eV.</td>
</tr>
<tr>
<td>00990</td>
<td>V(L) = longitudinal sound velocity as a function of (x).</td>
</tr>
<tr>
<td>01000</td>
<td>V(T) = transverse sound velocity as a function of (x).</td>
</tr>
<tr>
<td>01030</td>
<td>M00 = Te mass in amu</td>
</tr>
<tr>
<td>01040</td>
<td>M1 = Hg mass in amu</td>
</tr>
<tr>
<td>01050</td>
<td>M2 = Cd mass in amu</td>
</tr>
<tr>
<td>01060</td>
<td>PHI = mass density</td>
</tr>
<tr>
<td>01070</td>
<td>AL = lattice constant as a function of (x).</td>
</tr>
<tr>
<td>01110</td>
<td>EDISEV = disorder energy in eV.</td>
</tr>
<tr>
<td>01120</td>
<td>EDIS = disorder energy in ergs.</td>
</tr>
<tr>
<td>01140 to</td>
<td>EPHI0, EPHI1, EPHI2 are deformation potentials in ergs.</td>
</tr>
<tr>
<td>01160</td>
<td></td>
</tr>
</tbody>
</table>

93
<table>
<thead>
<tr>
<th>Line no.</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>01170</td>
<td>E1S = optical phonon scattering contribution.</td>
</tr>
<tr>
<td>01180</td>
<td>E2S = optical phonon scattering contribution.</td>
</tr>
<tr>
<td>01190</td>
<td>M1B = reduced mass.</td>
</tr>
<tr>
<td>01200</td>
<td>M2B = reduced mass.</td>
</tr>
<tr>
<td>01210</td>
<td>VA = the lattice constant cubed divided by 4.</td>
</tr>
<tr>
<td>01220</td>
<td>WL1 = longitudinal optical (LO) phonon frequency (HgTe), $k_B \theta_{E1}/\hbar$, where $\theta_{E1} = \text{LO phonon temperature}$.</td>
</tr>
<tr>
<td>01230</td>
<td>WL2 = longitudinal optical phonon frequency (CdTe), $k_B \theta_{E2}/\hbar$, where $\theta_{E2} = \text{LO phonon temperature}$.</td>
</tr>
<tr>
<td>01280</td>
<td>$E_G = E_g$ (ergs) as a function of $x$ and $T$ (temperature).</td>
</tr>
<tr>
<td>01285</td>
<td>$P = \text{momentum matrix element coupling conduction and valence bands (eV-cm) as a function of } x$.</td>
</tr>
<tr>
<td>01290</td>
<td>DELTA = $E_g$ divided by the spin-orbit splitting.</td>
</tr>
<tr>
<td>01330</td>
<td>SECULAR = an external program for finding the limit $E = E(k)$ at the zone boundary.</td>
</tr>
<tr>
<td>01370</td>
<td>$CON = \frac{2e^2}{\pi^2} \left( \frac{2\mu' m_0}{\hbar^2} \right)^{3/2} \left( \frac{k_B T}{\beta} \right)^{1/2}$, a factor that enters into Fermi-Thomas momenta expressions, i.e., $(k_{FT}^e)^2$, $(k_{FT}^{th})^2$, and $(k_{FT}^{hh})^2$.</td>
</tr>
<tr>
<td>01780</td>
<td>SIMP = an external program for evaluating integrals.</td>
</tr>
<tr>
<td>01790</td>
<td>KFTE2 = electron Fermi-Thomas momentum.</td>
</tr>
<tr>
<td>01810</td>
<td>KFTLH2 = light-hole Fermi-Thomas momentum.</td>
</tr>
<tr>
<td>01820</td>
<td>KFTTH2 = heavy-hole Fermi-Thomas momentum.</td>
</tr>
<tr>
<td>01840</td>
<td>THETA1 = $\theta_{E1}/T$ (see line no. 01220).</td>
</tr>
<tr>
<td>01850</td>
<td>THETA2 = $\theta_{E2}/T$ (see line no. 01230).</td>
</tr>
<tr>
<td>01860</td>
<td>GINF2 = $g_{inf}^2$, a parameter involving Fermi-Thomas momenta.</td>
</tr>
<tr>
<td>01870</td>
<td>GO2 = $g_{o2}^2$, a parameter involving Fermi-Thomas momenta.</td>
</tr>
<tr>
<td>01890</td>
<td>A1 = longitudinal optical (LO) phonon scattering contribution.</td>
</tr>
<tr>
<td>01910</td>
<td>A2 = acoustic phonon (ac) scattering contribution.</td>
</tr>
<tr>
<td>01930</td>
<td>A3 = ionized impurity (ii) scattering contribution.</td>
</tr>
<tr>
<td>01950</td>
<td>A4 = electron-hole (eh) scattering contribution.</td>
</tr>
<tr>
<td>01960</td>
<td>A5 = disorder scattering (dis.) contribution.</td>
</tr>
<tr>
<td>01980</td>
<td>NP1 = phonon-occupation number.</td>
</tr>
<tr>
<td>01990</td>
<td>NP2 = phonon occupation number.</td>
</tr>
<tr>
<td>02150</td>
<td>Q1 = $\lambda_1$ (matrix element).</td>
</tr>
<tr>
<td>02160</td>
<td>Q2 = $\lambda_2$ (matrix element).</td>
</tr>
<tr>
<td>Line no.</td>
<td>Comments</td>
</tr>
<tr>
<td>---------</td>
<td>----------</td>
</tr>
<tr>
<td>02170</td>
<td>$Q_3 = \mathcal{L}_3$ (matrix element).</td>
</tr>
<tr>
<td>02200</td>
<td>$Q_1 = (\mathcal{L}, \xi)_1$ (matrix element).</td>
</tr>
<tr>
<td>02210</td>
<td>$Q_2 = (\mathcal{L}, \xi)_2$ (matrix element).</td>
</tr>
<tr>
<td>02260</td>
<td>$\Sigma$ = conductivity.</td>
</tr>
<tr>
<td>02270</td>
<td>$U_H$ = Hall mobility.</td>
</tr>
<tr>
<td>02280</td>
<td>$\text{EGOPT} = k_B T / \beta$.</td>
</tr>
</tbody>
</table>
### Description of Symbols - Subroutine Programs

<table>
<thead>
<tr>
<th>Line no.</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. 02520</td>
<td>SECULAR - The program used to find the roots (E₁, E₂, E₃) of the cubic secular equation describing the conduction band, light-hole band, and split-off valence band.</td>
</tr>
<tr>
<td>B. 02700</td>
<td>CUBE - A subroutine for finding the roots of a cubic equation ( x^3 + c_2x^2 + c_1x + c_0 = 0 ).</td>
</tr>
<tr>
<td>B. 02700</td>
<td>FUNC - The program used to find the carrier concentration (electrons, light-holes, and heavy-holes) as a function of temperature.</td>
</tr>
<tr>
<td>B. 02700</td>
<td>SIMP - A subroutine used for evaluating a certain class of integrals.</td>
</tr>
<tr>
<td>02710</td>
<td>NE = electron concentration.</td>
</tr>
<tr>
<td>02780</td>
<td>NLH = light-hole concentration.</td>
</tr>
<tr>
<td>02800</td>
<td>NHH = heavy-hole concentration.</td>
</tr>
<tr>
<td>C. 03000</td>
<td>FV - The program used to obtain the Fermi distribution function</td>
</tr>
<tr>
<td>D. 03000</td>
<td>FUNC1 - The program used to obtain the product FV and LAMDA.</td>
</tr>
<tr>
<td>D. 03000</td>
<td>LAMDA - A function used to calculate the conduction band density-of-states.</td>
</tr>
<tr>
<td>D. 03080</td>
<td>FUNC2 - The program used to obtain the product of FV and LAMDAV.</td>
</tr>
<tr>
<td>D. 03080</td>
<td>LAMDAV - A function used to calculate the light-hole density-of-states.</td>
</tr>
<tr>
<td>D. 03080</td>
<td>FVP - This program evaluates the function ( \exp(y + z) / [\exp(y + z) + 1]^2 ).</td>
</tr>
<tr>
<td>D. 03080</td>
<td>FUNC3 - This program evaluates the function ( \lambda_c \exp(y - z) / [\exp(y + z) + 1]^2 ).</td>
</tr>
<tr>
<td>D. 03080</td>
<td>FUNC4 - This program evaluates the function ( \lambda_{ph} \exp(y - z) / [\exp(y + z) + 1]^2 ).</td>
</tr>
<tr>
<td>D. 03080</td>
<td>LAMDA = ( \lambda_c ), an expression used in calculating the conduction-band density-of-states.</td>
</tr>
<tr>
<td>D. 03080</td>
<td>LAMDAV = ( \lambda_{ph} ), an expression used in calculating the light-hole density-of-states.</td>
</tr>
<tr>
<td>D. 03080</td>
<td>S - This program evaluates a function used in determining the crystal momentum.</td>
</tr>
<tr>
<td>D. 03080</td>
<td>L1 - This program evaluates ( L^{(n)} ).</td>
</tr>
<tr>
<td>D. 03080</td>
<td>NABC - This program evaluates the function ( F_\lambda(y) ), which appears in the LO-phonon scattering operator ( q_{LO} ).</td>
</tr>
<tr>
<td>D. 03080</td>
<td>RSL - This program evaluates functions appearing in the LO-phonon scattering operator.</td>
</tr>
<tr>
<td>04390</td>
<td>ROP1 = ( \rho^+_0(y, \theta_1) )</td>
</tr>
<tr>
<td>04410</td>
<td>ROP2 = ( \rho^+_0(y, \theta_2) )</td>
</tr>
<tr>
<td>04440</td>
<td>ROM1 = ( \rho^-_0(y, \theta_1) )</td>
</tr>
<tr>
<td>04470</td>
<td>ROM2 = ( \rho^-_0(y, \theta_2) )</td>
</tr>
<tr>
<td>04530</td>
<td>R1P1 = ( \rho^+_1(y, \theta_1) )</td>
</tr>
<tr>
<td>04540</td>
<td>R2P1 = ( \rho^+_2(y, \theta_1) )</td>
</tr>
<tr>
<td>04590</td>
<td>R1P2 = ( \rho^+_1(y, \theta_2) )</td>
</tr>
<tr>
<td>04600</td>
<td>R2P2 = ( \rho^+_2(y, \theta_2) )</td>
</tr>
<tr>
<td>04680</td>
<td>R1M1 = ( \rho^-_1(y, \theta_1) )</td>
</tr>
<tr>
<td>04670</td>
<td>R2M1 = ( \rho^-_2(y, \theta_1) )</td>
</tr>
<tr>
<td>04730</td>
<td>R1M2 = ( \rho^-_1(y, \theta_2) )</td>
</tr>
<tr>
<td>Line no.</td>
<td>Comments</td>
</tr>
<tr>
<td>---------</td>
<td>----------</td>
</tr>
<tr>
<td>04740</td>
<td>( R_{2M2} = p_2^- (v, \theta_2) )</td>
</tr>
<tr>
<td>04760</td>
<td>( \Sigma Y_2 = s^2 )</td>
</tr>
<tr>
<td>04770</td>
<td>( Q_1P = q_1^+ )</td>
</tr>
<tr>
<td>04780</td>
<td>( Q_2P = q_2^+ )</td>
</tr>
<tr>
<td>04800</td>
<td>( Q_1M = q_1^- )</td>
</tr>
<tr>
<td>04820</td>
<td>( Q_2M = q_2^- )</td>
</tr>
<tr>
<td>04840</td>
<td>( P_{1P} = P_1^+ )</td>
</tr>
<tr>
<td>04850</td>
<td>( P_{2P} = P_2^+ )</td>
</tr>
<tr>
<td>04870</td>
<td>( P_{1M} = P_1^- )</td>
</tr>
<tr>
<td>04890</td>
<td>( P_{2M} = P_2^- )</td>
</tr>
<tr>
<td>04910</td>
<td>( V_{1P} = r_1^+ )</td>
</tr>
<tr>
<td>04920</td>
<td>( V_{2P} = r_2^+ )</td>
</tr>
<tr>
<td>04940</td>
<td>( V_{1M} = r_1^- )</td>
</tr>
<tr>
<td>04960</td>
<td>( V_{2M} = r_2^- )</td>
</tr>
<tr>
<td>05000</td>
<td>( V_{0P1} = V_0^+ (v, \theta_1) )</td>
</tr>
<tr>
<td>05010</td>
<td>( V_{1P1} = V_1^+ (v, \theta_1) )</td>
</tr>
<tr>
<td>05020</td>
<td>( V_{2P1} = V_2^+ (v, \theta_1) )</td>
</tr>
<tr>
<td>05040</td>
<td>( V_{3P1} = V_3^+ (v, \theta_1) )</td>
</tr>
<tr>
<td>05090</td>
<td>( V_{0P2} = V_0^+ (v, \theta_2) )</td>
</tr>
<tr>
<td>05100</td>
<td>( V_{1P2} = V_1^+ (v, \theta_2) )</td>
</tr>
<tr>
<td>05110</td>
<td>( V_{2P2} = V_2^+ (v, \theta_2) )</td>
</tr>
<tr>
<td>05130</td>
<td>( V_{3P3} = V_3^+ (v, \theta_2) )</td>
</tr>
<tr>
<td>05190</td>
<td>( V_{0M1} = V_0^- (v, \theta_1) )</td>
</tr>
<tr>
<td>05200</td>
<td>( V_{1M1} = V_1^- (v, \theta_1) )</td>
</tr>
<tr>
<td>05210</td>
<td>( V_{2M1} = V_2^- (v, \theta_1) )</td>
</tr>
<tr>
<td>05230</td>
<td>( V_{3M1} = V_3^- (v, \theta_1) )</td>
</tr>
<tr>
<td>05290</td>
<td>( V_{0M2} = V_0^- (v, \theta_2) )</td>
</tr>
<tr>
<td>05300</td>
<td>( V_{1M2} = V_1^- (v, \theta_2) )</td>
</tr>
<tr>
<td>05310</td>
<td>( V_{2M2} = V_2^- (v, \theta_2) )</td>
</tr>
<tr>
<td>05330</td>
<td>( V_{3M2} = V_3^- (v, \theta_2) )</td>
</tr>
<tr>
<td>05390</td>
<td>( R_{P1} = R_+ (v, \theta_1) )</td>
</tr>
<tr>
<td>05400</td>
<td>( S_{P1} = S_+ (v, \theta_1) )</td>
</tr>
<tr>
<td>05430</td>
<td>( R_{P2} = R_+ (v, \theta_2) )</td>
</tr>
<tr>
<td>05440</td>
<td>( S_{P2} = S_+ (v, \theta_2) )</td>
</tr>
<tr>
<td>05480</td>
<td>( R_{M1} = R_- (v, \theta_1) )</td>
</tr>
<tr>
<td>Line No.</td>
<td>Comments</td>
</tr>
<tr>
<td>---------</td>
<td>----------</td>
</tr>
<tr>
<td>05490</td>
<td>SM1 = S (v, \theta_1)</td>
</tr>
<tr>
<td>05560</td>
<td>RM2 = R (v, \theta_2)</td>
</tr>
<tr>
<td>05570</td>
<td>SM2 = S (v, \theta_2)</td>
</tr>
<tr>
<td>05620</td>
<td>PI0 = \pi_0 (y)</td>
</tr>
<tr>
<td>05640</td>
<td>PI2 = \pi_2 (y)</td>
</tr>
<tr>
<td>05690</td>
<td>PHI0 = \phi_0 (y)</td>
</tr>
<tr>
<td>05710</td>
<td>PHI1 = \phi_1 (y)</td>
</tr>
<tr>
<td>05730</td>
<td>PHI2 = \phi_2 (y)</td>
</tr>
<tr>
<td>05770</td>
<td>PHI = \Phi</td>
</tr>
<tr>
<td>05810</td>
<td>A1 = A_1 (y)</td>
</tr>
<tr>
<td>05820</td>
<td>A2 = A_2 (y)</td>
</tr>
<tr>
<td>05830</td>
<td>A3 = A_3 (y)</td>
</tr>
<tr>
<td>05840</td>
<td>A4 = A_4 (y)</td>
</tr>
<tr>
<td>05850</td>
<td>B1 = B_1 (y)</td>
</tr>
<tr>
<td>05880</td>
<td>B2 = B_2 (y)</td>
</tr>
<tr>
<td>05890</td>
<td>B3 = B_3 (y)</td>
</tr>
<tr>
<td>05900</td>
<td>B4 = B_4 (y)</td>
</tr>
<tr>
<td>05910</td>
<td>B5 = B_5 (y)</td>
</tr>
<tr>
<td>05930</td>
<td>B6 = B_6 (y)</td>
</tr>
<tr>
<td>05940</td>
<td>FLY = F_L (y)</td>
</tr>
<tr>
<td>05960</td>
<td>FTY = F_T (y)</td>
</tr>
<tr>
<td>3010</td>
<td>LB = L_B (y)</td>
</tr>
<tr>
<td>P.</td>
<td>ROOT - This program calculates limits.</td>
</tr>
<tr>
<td>Q.</td>
<td>INTEG - This program evaluates integrals.</td>
</tr>
<tr>
<td>R.</td>
<td>FMN - This program calculates the elements of the determinant F_{mn} (y).</td>
</tr>
<tr>
<td>S.</td>
<td>FM - This program evaluates a function involving FVP and L1.</td>
</tr>
<tr>
<td>T.</td>
<td>HCSPOL - This program calculates as a function of x, the TO and LO phonon temperature, the transverse effective charges, the Callen effective charges, and the dielectric constants \epsilon_0 and \epsilon_\infty.</td>
</tr>
<tr>
<td>07520</td>
<td>ESTR1 = HgTe transverse charge.</td>
</tr>
<tr>
<td>07530</td>
<td>ESTR2 = CdTe transverse charge.</td>
</tr>
<tr>
<td>07531</td>
<td>XM1 = HgTe reduced mass in g.</td>
</tr>
<tr>
<td>07532</td>
<td>XM2 = CdTe reduced mass in g.</td>
</tr>
<tr>
<td>07533</td>
<td>A = lattice constant as a function of x.</td>
</tr>
<tr>
<td>07540</td>
<td>EPS1 = \epsilon_\infty as a function of x.</td>
</tr>
<tr>
<td>07550</td>
<td>EPS0 = \epsilon_0 as a function of x.</td>
</tr>
<tr>
<td>Line No.</td>
<td>Comments</td>
</tr>
<tr>
<td>---------</td>
<td>----------</td>
</tr>
<tr>
<td>07560</td>
<td>( W_T = \omega_T (CdTe) ) as a function of ( x ).</td>
</tr>
<tr>
<td>07570</td>
<td>( W_T = \omega_T (HgTe) ) as a function of ( x ).</td>
</tr>
<tr>
<td>07630</td>
<td>( THT1 = HgTe ) TO - phonon temperature.</td>
</tr>
<tr>
<td>07640</td>
<td>( THT2 = CdTe ) TO - phonon temperature.</td>
</tr>
<tr>
<td>07791</td>
<td>( THT1 = HgTe ) LO - phonon temperature.</td>
</tr>
<tr>
<td>07782</td>
<td>( THT2 = CdTe ) LO - phonon temperature</td>
</tr>
<tr>
<td>07860</td>
<td>( EC1 = ) Callen effective charge for HgTe.</td>
</tr>
<tr>
<td>07870</td>
<td>( EC2 = ) Callen effective charge for CdTe.</td>
</tr>
</tbody>
</table>
```
IF(NRUN.EQ.1)
    T
    GO TO 21
    WRITE(6,31)
    3
    CONTINUE I=YES, 2=NO
    READ(2,1) NCONT
    IF(NCONT.EQ.2)
        T
        GO TO 550
    21
    NRUN=NRUN+1
    WRITE(6,41)
    WRITE(6,31)
    FORMAT(ENTER NUMBER OF PAMS TO BE CHANGED AND I.
          FOR EACH CHANG: E)
    READ(2,1) NCHNGE, (ISBSCP(I), VALUE(I), I=1, NCHNGE)
    DO 25 I=1, NCHNGE
       J=ISBSCP(I)
 25      CONT. ON PG 3
```
CON=CON*Sqrt(CL); I
Z=1000./T
DELT=0.3*I
GEND=.FALSE.

70
XDL=FUNC(2)

IF XDL.LT.0.0)

T
GO TO 75

GEND=.TRUE.
XDL=XDL
Z=Z-DELT
GO TO 70

75
IF(GEND)

T
GO TO 90

GO TO 85

GO TO 85

XDL=XDU

CON ON PG 6
$S$, $A4$

$Z = Z + \text{DELZ}$

$\text{ADU} = \text{FUNC}(Z)$

IF $\text{ADU} \lt \text{LT} \cdot 0.01$

$T$

GO TO 20

$ZU \div 2$

$ZL = Z - \text{DELZ}$

GO TO 35

$S$, $A5$

$ZL = Z$

$ZU = Z - \text{DELZ}$

GO TO 65

IF (DELZ - LE.2 - E - 4 * ABS(Z))

$T$

GO TO 110

DELZ = DELZ / 2.

Z = ZL + DELZ

XOM = FUNC(Z)

CONT. ON PG
SUBROUTINE SECULAR(KS,E1,E2,E3)

REAL KT,ND,MD,NA
REAL KS
COMMON /CONST/ PI,P,HB,KT,ND,UV,MD,EG,YBC,YBV,NA,ZI,ZA
C0=P*KS
C2=0-EG
C1=-EG+D+CO
CO=-2.*D*CO/3.

CALL CUBE(C2,C1,CO,E1,E2,E3)

RETURN

END

ORIGINAL PAGE IS
OF POOR QUALITY
FUNCTION FUNC1(X)

REAL NE, NLH, NHM
REAL KT, ND, MO, NA
REAL NOD, ND1
COMMON/CONST1/PI,P,HB,KT,ND,UV,MO,DEG,YBC,YBV,WA,ZI,ZA
COMMON/NNN/NE,NLMH,NHM,ND1
COMMON/VAR/Z,CON
COMMON/CONST2/BETA,DELTA,BI
EXTERNAL FUNC1,FUNC2

NE=0.0
X2=10.+BI

IF(Z.GT.BI)
F

T

X2=10.+Z

X2=AMINI(YBC,X2)

IF(X2.LE.BI)
F

T

GO TO 100

CALL SIMPLFUNC1,BI,X2,0.01,10,SI1,NE,N,IER

NE=CONNE

100

CONT. ON PG 2
X2 = 10.

IF(Z.LT.0.0)

T

X2 = (10. - Z)

F

X2 = AMIN1(YB, X2)

IF(X2.LE.0.0)

T

GO TO 200

CALL SIMP(FUNC2.0,0,X2,0,0,1,0,SII,NLH,N,IER)

NLH = CON*NLH

GO TO 200

NHM = NHM + F(1. - Z)/(2.*PI*PI)

ED = 0.003*1.60219*17E-12

E2 = E0 - ED

NDD = 1.0*E0/(0.5*EXP(-E2/KT*Z) + 1.0)

ND1 = ND1 + NDD

FUNC = NE - NLH - NHM - ND1*Z1 + NA*ZA

RETURN

END
FUNCTION FV(Y,Z)

IF(Y+Z.LE.500.)

T

GO TO 10

IF(Y+Z.LE.500.)

T

GO TO 20

FV=0.0

GO TO 30

10

FV=1.0

GO TO 30

20

FV=1.0/(EXP(Y+Z)+1.)

30

CONTINUE

RETURN

END
FUNCTION FUNC1(Y)

REAL LAMDA
COMMON /VAR/ Z, CON
FUNC1=FV(Y, -Z) * LAMDA(Y)

RETURN

END

FUNCTION FUNC2(Y)

REAL LAMDAV
COMMON /VAR/ Z, CON
FUNC2=FV(Y, Z) * LAMDAV(Y)

RETURN

END
FUNCTION FUNC3(Y)

REAL LAMDA
COMMON /VAR/ Z, CON
FUNC3 = LAMDA(Y) * FYP(Y, -Z)

RETURN

END

FUNCTION FUNC4(Y)

REAL LAMDAV
COMMON /VAR/ Z, CON
FUNC4 = LAMDAV(Y) * FYP(Y, Z)

RETURN

END
REAL FUNCTION LAMBDA(I)

COMMON /CONST2/ BETA, DELTA, BI BY=DETA+Y

IF(Y.EQ.BI)

T

BY=1.

LAMDA=2.*DELTA+DELTA*B*BY+BY+DELTA*(3.-DELTA)*BY+BY +4.*((1.-DELTA)*BY/3.-2./3.

X=3.*DELTA+BY/2.+1.
LAMDA=3.*LAMDA*SORRT*(BY+1.)/((DELTA+BY-1.)/((X*X*X*X*X)/2.

RETURN

END

REAL FUNCTION LAMDA(Y)

COMMON /CONST2/ BETA, DELTA, BI BY=DETA+Y

LAMDA=2.*DELTA+DELTA*B*BY+BY-DELTA*(3.-DELTA)*BY+BY +4.*((1.-DELTA)*BY/3.-2./3.

X=3.*DELTA+BY/2.-1.
LAMDA=3.*LAMDA*SORRT*(BY+1.)/((DELTA+BY-1.)/((X*X*X*X*X)/2.

RETURN

END
C

FUNCTION S(Y)

C

COMMON /CONST2/ BETA, DELTA, BI
BI=BETA+Y

IF(Y.EQ.BI)

T

BY=1.

S=SQRT(BY*(BY-1.)*(DELTA*BY-1.)/((3.*DELTA*BY/2.+1.)))

RETURN

END

C

REAL FUNCTION LI(Y)

C

COMMON /CONST2/ BETA, DELTA, BI
LI=S(Y)/SQRT(BETA)
LI=L1*L1*L1

RETURN

END
FUNCTION H(Y,THETA)
C

H=0.0

IF(Y.LT.THETA) F
T
RETURN

H=1.0
RETURN

END

PG. 1 FINISH
SUBROUTINE NABC(Y, A, B, BP, C, CP, FL)

REAL N
COMMON /CONSTR/ BETA, DELTA, BI
BY = BETA, Y

IF(Y.EQ.BI):

T

BY = 1.

DBY = DELTA * BI

DBY23 = DBY + 2. / 3.
N = SORT (BY * (DBY + 1.) * DBY23 + 2. * (BY - 1. / 9.) + (BY - 1.) * DBY23 * DBY23)
A = SORT (BY * (DBY + 1.) * DBY23 / N
B = SORT (2. * (BY - 1. / 1.)) / (3. * N)
C = SORT (1. * DBY23 / N)
CP = SORT (3. * DBY / 2. + 1.) / (BY * (DBY + 1.))
BP = SORT (2. * CP / (3. * N)
CP = DBY23 * CP / N


RETURN

END

ORIGINAL PAGE IS OF POOR QUALITY
SUBROUTINE RSL(Y,RP1,RP2,RM1,RM2,SP1,SP2,SM1,SM2,LB)

REAL LAMDA
REAL LB
COMMON /CONST2/ BETA,DELTA,BI
COMMON /CONST3/ THETA1,THETA2,GINF2,GO2,EPHI0,EPHI1,EPHI2,
                 VL,VT,SP2,SA3,SA4,SA5

YM1B=Y-THETA1-BI
YM2B=Y-THETA2-BI
SY=S(Y)
SP1=S(Y+THETA1)
SP2=S(Y+THETA2)

IF(YM1B.LT.0.0)
   F
   T
   GO TO 10

SM1=S(Y-THETA1)

10

IF(YM2B.LT.0.0)
   F
   T
   GO TO 20

SM2=S(Y-THETA2)

CONT. ON PG 2
\[
V2M = (VIM + (1 - 2 \times PIM/\text{QIM} + (1 - PIM/\text{QIM}) \times PIM + PV) \\
\times PIM + (2 - 3 \times PIM/\text{QIM}) \times X/2) 	imes 1/4.
\]

\[
V3M = -VIM \times VIM \times VIM/\text{QIM} + PIM \times VIM \\
\times (1 - 3 \times PIM/\text{QIM} + PIM \times PIM/\text{QIM} + PV) \\
\times (1 - PIM \times PIM/\text{QIM} + PV) \\
\times (2 - 4 \times PIM/\text{QIM} \times X/16).
\]

\[
X = \text{ALGOABS}(P2M - 2 \times V2M)/(P2M + 2 \times V2M)
\]

\[
V2M = V2M + (P2M + 4 \times V2M) \\
VIM = (1 - 2 \times P2M/\text{Q2M} + (1 - P2M/\text{Q2M}) \times P2M + PV) \\
\times P2M + (2 - 3 \times P2M/\text{Q2M}) \times X/2) \times 1/4.
\]

\[
V3M = -V2M \times V2M \times V2M/\text{Q2M} + P2M \times V2M \\
\times (1 - 3 \times P2M/\text{Q2M} + P2M \times P2M/\text{Q2M} + PV) \\
\times (1 - P2M \times P2M/\text{Q2M} + PV) \\
\times (2 - 4 \times P2M/\text{Q2M} \times X/16).
\]
ORIGINAL PAGE IS OF POOR QUALITY
ORIGINAL PAGE IS OF POOR QUALITY

IF (B - A.LT.TOL) THEN
  T
  RETURN
ELSE
  GO TO 7
ENDIF

A2

30

A3

10C

RETURN

END
GO TO 100

A2

DEL = 0.0001 \times (B - R)

Y = R

X = Y - DEL

DEL = 5 \times DEL

IF (X < T)

F

T

X = A

CALL SIMP(F, X, Y, 0, 0, 10, SP, VAL, N, IE)

WRITE(B, X, Y, SP, VAL, N, IE)

V = V + VAL

IF (X = A)

F

T

RETURN

Y = X

GO TO 300

END

PG 2 FINAL

135
FUNCTION FMH(Y)

REAL LB.NP1.NP2
COMMON /VAR/ Z.CON
COMMON /NM/ N.M
COMMON /CONST2/ BETA.DELTA.BI


COMMON /CONST4/ NP1.NP2.X1.X2.AI
   X=1-BI

CALL RSL(Y.RP1.RP2.RM1.RM2.SP1.SP2.SM1.SM2.LB)

XM=0.0
XN=0.0

IF(X.EQ.0.0)

T

GO TO 10

XM=XM*XM
XN=XN*XN

10

XMN=XM*XN

XFIN=(X+THETA1)**N
XP2N=(X+THETA2)**N
XM1N=0.0
XM2N=0.0

CONT. ON PG 2
IF (X-THETA1.LE.0.0)  

IF (X-THETA2.LE.0.0)  

XMIN=(1.-THETA1)**N  

XM2N=(X-THETA2)**N  

FY=FV(Y,-Z)  

FMN=X1*B1*X2*(FV1*(Y-THETA1,-Z)*NP1+1.)*(XP1*RP1-XN*SP1)/FY  
+FV(Y-THETA1,-Z)*NP1*XY.Y,THETA1)*(XM1*RM1-XN*SM1)/FY  
+X2*A1*B1*XY.FV1*(Y+THETA2,-Z)*NP2+1.)*(XP2*RP2-XN*SP2)/FY  
+FV(Y-THETA2,-Z)*NP2*XY.Y,THETA2)*(XM2*RM2-XN*SM2)/FY  
-LB*XMN  

FMN=-FMNFVF(Y,-Z)  

RETURN  

END
FUNCTION FM(Y)

REAL LI
COMMON / VAR / Z,CON
COMMON / NM / N.M
COMMON / Const2 / BETA,DELT.A.BI
X=Y-BI
XM=D.B.

IF(X.EQ.0.D.)

IF

GO TO 10

XM=X*M

CONTINUE

FM=-FVP(Y,-Z)*LI(Y)*XM

RETURN

END
SUBROUTINE HCSPOLI(X,THT1,THT2,THL1,THL2,ESTP1,ESTR2,EPSO,
EPS1,EC1,EC2)

ESTR1=2.96
ESTR2=2.35
XM1=-29850*E-22
XM2=9.9239*E-23
A=(6.460*E-21)*X*1.0E-8
ESTP1=15.1077*E-21*8.88928*X*X*X=3.47133*X*X*X
ESTR=20.286*E-15.1531*E-6.53091*X*X*X=0.961326*X*X*X
WT2=5.20-9.0*E

WT1=118.0+12.0*E
ES=4.86325*E-10
HB=1.054591*E-27
EK=1.380622*E-16
LI=3.141593
C=2.9979250E10
THT1=2.*P1*X*HB/MB*WT1
THT2=2.*P1*X*HB/MB*WT2

OMT1=8K*THT1/KB
OMT2=8K*THT2/KB
F1=4.4*P1/(X/0.04*K)*ESTR1*X/2./XM1*(J:.-)*ESTR2*X/2./XM2*X/ES*X
S1=F1/OMT1*X
S2=F2/OMT2*X

THLM2=1./2./*EPS1*EPS1*THT1*X/2.+THT2*X/2.+S1*THT1*X/2.
+2*THT2*X/2.-SORT(T1EPS1*THT2*X/2.-THT1*X/2.)*S1*THT1*X/2.
-S1*THT1*X/2.)*S1*THT1*X/2.*THT2*X/2.*S1*X/2.

THLP2=1./2./*EPS1*EPS1*THT1*X/2.+THT2*X/2.+S1*THT1*X/2.
+S2*THT2*X/2.-SORT(T1EPS1*THT2*X/2.-THT1*X/2.)*S2*THT1*X/2.
-S1*THT1*X/2.)*S1*THT1*X/2.*THT2*X/2.*S1*X/2.

THLD=SORT((1EPS1+S1)/EPS1*THT1
TML2=THLM2
THL2=THLP2

IF(THT2.GT.THLD)
  T
  GO TO 10
  R1
  TML2=THLP2

CONT. ON PG 2
ORIGINAL PAGE IS OF POOR QUALITY

142
06680 XZ=AMIN1(YBC,X2)
06690 IF(XZ<=LE.B) GO TO 100
07700 CALL SIMP(FUNCI,81,0,0.01,10,Sl1,NE,N+1,IER)
02710 NE=CN+NE
02720 100 NLH=N
02730 XZ=X
02740 IF(I*LT+0.0) XZ=(10.*Z)
02750 IF(XZ<=LE.B) GO TO 200
02760 CALL SIMP(FUNC2,81,0,0.01,10,Sl1,NE+N+I,IER)
02770 NLH=CON+NLH
02780 200 NLH=NLH+(3.*VAV*KT)/(12.*EPR*VAV)
02800 NHA=NLH*F[(1-2)*12.*EPR]
02801 ED=0.003*1.6021972E-12
02802 E2=E0+ED
02803 EDD=l.OE9/(E2/EK+2+1.*0)
02804 NUL=ND*EDD
02810 FUNC=NLH-NHH-ND1*Z1+NA*Z
02820 RETURN
02830 END
02840C FUNCTION FV(Y,Z)
02850C
02860C IF(Y*Z.LE.500.) GO TO 10
02870 YZ=500.1 GO TO 20
02880 FV=0.
02890 GO TO 30
02900 FV=1.
02910 GO TO 30
02920 FV=Y/EXP(Y+Z)+1.
02930 C CONTINUE
02940 RETURN
02950 END
02960C FUNCTION FUNC1(Y)
02970C
02980 REAL LAMDA
03000 COMMON /VAR/ Z, CON
03020 FUNC1=FV(Y,=)*LAMDA(Y)
03040 RETURN
03050C
03060C REAL LAMDA
03080 COMMON /VAR/ Z, CON
03090 FUNC2=FV(Y,=)*LAMDAV(Y)
03100 RETURN
03120 END
03130C FUNCTION FVP(Y,Z)
03140C
03150C IF(Y*Z.LE.200.) GO TO 10
03170 IF(Y*Z.LE.200.) GO TO 20
03180 FVP=0.
03190 GO TO 30
03200 FVP=0.
03210 GO TO 30
03220 FVP=EXP(Y+Z)
03230 FVP=FVP/(FVP+1.)/(FVP+1.)
03250 C CONTINUE
03260 RETURN
03260C END
03270C FUNCTION FUNC3(Y)
03280C
03290C REAL LAMDA
03310 COMMON /VAR/ Z, CON
03320 FUNC3=LAMDAV(Y)*FVP(Y,=)
03330 RETURN
03340 END
03350C FUNCTION FUNC4(Y)
03360C
03370C REAL LAMDA
03390 COMMON /VAR/ Z, CON
03400 FUNC4=LAMDAV(Y)*FVP(Y,=)
03410 RETURN
03420 END
03430C REAL FUNCTION LAMDA(Y)
03450C COMMON /CONST2/ BETA, DELTA, BI
03470 BT=BLTA+T
REAL FUNCTION LAMDAV(Y)

COMMON /CONST2/ BETA,DELTABY1
LAMDAV=2.*DELTABY*BY*BY*BY*BY
RETURN
END

FUNCTION SIGM(Y)

BY=BETA-Y
IF(Y.LT.BY)
RETURN
GEBY = SQRT(BY)
END

REAL FUNCTION L1(Y)

COMMON /CONST2/ BETA,DELTABY1
L1=Y/SQRT(BETA)
RETURN
END

FUNCTION M(Y,THETA)

M=0.0
IF(Y.LT.THETA) RETURN
M=1.0
RETURN
END

SUBROUTINE NABC(Y,A,B,C,P,FL)

REAL N
COMMON /CONST2/ BETA,DELTABY1
BY=DELTABY*BY
N=SQRT((BY+1./3.)*DBY23+DBY23)/DBY23
RETURN
END

SUBROUTINE RSL(Y,RP1,RP2,RM1,RM2,SP1,SP2,SM1,SM2,SL)

REAL LAMDA
COMMON /CONST2/ BETA,DELTABY1
LAMDA=2.*DELTABY*BY*BY*BY*BY*BY
RETURN
END

CONTINUE
CALL NABC(Y,A,B,C,P,FL)
CALL NABC(Y,THETA1,AP1,BP1,CP1,PP1,FLP1)
CALL NABC(Y,THETA2,AP2,BP2,CP2,PP2,FLP2)

IF (YH2.LT.0) GO TO 30
CALL NABC(Y-THETA,AM,BP,BU,CY,CP,FLM)
GO TO 30

CONTINUE
IF (YH2.LT.0) GO TO 30
CALL NABC(Y-THETA,AM,BP,BU,CY,CP,FLM)

CONTINUE
0530 CONTINUE
BC=CP*CP
RGP=R1*CP+1*BP*BC/S2+BC/2+8*BP1/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
RGP=R1*BP2*BP2=8*BP2/8+
SUBROUTINE ROOT(F, A, TOL)

2 = 1.0
FA = F(A)

IF(YEQTOL) GO TO 200
Z = A
RETURN
END

SUBROUTINE INTEGR(F, A, B, Y)

FUNCTION FMN(Y)

REAL LR, NP, NP1, NP2
COMMON /VAR/ ZE, CON
COMMON /NM/ N, NM
COMMON /CONST/ BETA, DELTA, B1
COMMON /CONST2/ BETA DELTA, B2, GINF, G02, EPSM1, EPSM2, EPSM2
COMMON /CONST3/ NP1, NP2, X1, X2, XA

XNa = Y - B1
CALL RSL(Y, RP1, RP2, RM1, RM2, SP1, SP2, SM1, SM2, LB)

XN = 0.0
XM = 0.0
XMN = 0.0
10 XM = XM + XN
XP1 = (X + THETA1)**N
XP2 = (X + THETA2)**N
XM = XM + XMN
XMN = XMN + XN
IF(X - THETA1EQB0) GO TO 20
XM = XM + XMN
IF(X - THETA2EQB0) GO TO 30
XM = XM + XMN
CONTINUE

F = FV(Y - Z)
FMN = FV(Y + THETA1 + Z) * (NP1 + 1) * (NP1 + RP1 - XM + SP1) / FV

4 = B2 * XN
FMN = FMN - FV(Y + Z)
RETURN
END
**FUNCTION FM(Y)**

**REAL**  
COMMON /VAR/ Z, CON  
COMMON /NM/ N, M  
COMMON /CONST2/ BETA, DELTA, BI  
XM = BI  
IF(X EQ 0.0) GO TO 10  
XM = XM  
**10 CONTINUE**  
FM = FP(Y, Z)*L1(Y)*XM  
RETURN  
END  

**SUBROUTINE MCSPOL(X, TH1, TH2, THL1, THL2, ESTR1, ESTR2, EPS0,**

**1 EPSI (E1, E2)**

**REAL** L1  
COMMON /VAR/ ZICON  
COMMON /NM/ NrM  
**OMWON** /CONSTZ/ BETA, DELTA, B1

**S. V-BI**  
**"X"**  
**CUBE (BrCrDrEI**

**CUBE** WRITTEN 9/19/74 JHP

**COMMENTS:**

**THIS ROUTINE SOLVES THE GENERAL CUBIC EQUATION**

**X** = 3 * X**2 + C**X + D = 0

**HAVING ONLY REAL SOLUTIONS E1 > E2 > E3.**

**IT IS ASSUMED THAT ALL SOLUTIONS ARE REAL.**

**REAL** E(3)  
**COMPLEX** X1, X2, X3, F, SO, Y, Z, S  
**= CMPLX(-5, 5)*SQRT(3.125)**

**PS = (B*B/3.125)**

**Q = (2*B*B/27) + (C*B/3.125)**

**F = (Q*Q + 4*P)**  
**= SQRT(F)**

**S = SQRT(2)**

**Y = 0.0**

**IF (ABS(S) .NE. 0.0) Y = CEXP(CLOG(S)/3.0)**
$S = -U - \frac{Q}{2}.$

IF(CABS(S) .NE. 0.0) Z = CEXP(CLOG(S)/3.).

X1 = Y - B/3.
X2 = Y + B/3.
X3 = X + B/3.

E(1) = HEAL(X1)
E(2) = HEAL(X2)
E(3) = HEAL(X3)
DO 100 I = 1, 12000
J = I + 1
100 IF(E(I) .LE. E(J)) GO TO 100

RETURN

ORIGINAL PAGE IS OF POOR QUALITY

FUNCTION F(K2 + ETA)
DIMENSION CON(4, S)
COMMON ETA, TABX(241), FTM12(241) + FT32(241) + FT52(241)
DATA CON / 1.7725393, 1.421361, 4.132332, -1.0756866
DATA A = 0.2522593, 0.284271, 1.2330051, 1.055719
DATA B = -0.3204029, -0.5366602, 0.1685927, -1.7756866
DATA L = -1.3231511, 1.31370814, 3.931713, 12.429809
DATA K = 1.63729, 22.627417, 25, 90.77111, 111.86825
RETURN

IF(X .GE. ETATAB(241)) GO TO 10

EXPX = X
IF(X .LE. 1E-20) GO TO 5

CALL INTPR(X, ETA, CFTAB, FTM12, FT32, FT52)
IF(I2O .EQ. 0) RETURN

FORMAT (*INTERPOLATION ERROR IN F(*, 12*, *2*, *101.5*, *11))
RETURN

END

SUBROUTINE INTRPL(X, TABX, TABY, NC, YPIND)
NC = INDEP VARIABLE
TABX = X ARRAY
TABY = Y ARRAY
NC = CONTROL WORD
TY = UNITS POSITION - DEGREE OF INTERPOLATION (1-7)
NC = INDEPENDENT VARIABLE RETURNED TO CALLING PROGRAM
NUMBER OF VALUES IN TABLE
DIMENSION TABX(NC), TABY(NC)
X = IABS(NC)
IF(KC .GE. 10) GO TO 65
RETURN

END

LAGRANGIAN INTERPOLATION ROUTINE
SUBROUTINE INTRPL(X, TABX, TABY, NC, YPIND)
NC = INDEPENDENT VARIABLE
TABX = X ARRAY
TABY = Y ARRAY
NC = CONTROL WORD
TY = UNITS POSITION - DEGREE OF INTERPOLATION (1-7)
NUMBER OF VALUES IN TABLE
DIMENSION TABX(NC), TABY(NC)
X = IABS(NC)
IF(KC .GE. 10) GO TO 65
RETURN

END
SUBROUTINE DISSESS(XA,TAB,NX,IND,NPX,KEY,NO)
DISSESS LOCATES XA IN TAB AND RETURNS WITH
LOWER LIMIT FOR SUMMATION. NO=1 IF ERROR
DIMENSION TAB(NX)
IF(XA<TAB(1)) 71,73,72
IF(XA<TAB(1)) 74
7 XA=TA(B(1))
74 NPX=1
RETURN
72 IF(XA<TAB(NX)) 1,77,76
76 NPX=NX-IND+1
71 IF(KEY.EQ.0) GOTO 74
73 XA=TA(B(NX))
72 IF NPX=NX-IND
50 RETURN
50 RETURN
74 IF DISSESS TAKES THIS PATH XA IS WITHIN RANGE OF TAB
1 OTHER CASES
IF(XA.EQ.TAB(NX)) GOTO 74
IF(XA.EQ.TAB(NX)) GOTO 74
74 NPX=NX-IND+1
RETURN
12 NPX=NX-IND+1
RETURN
77 IF(XA<TAB(NX)) GOTO 18
78 IF(XA<TAB(NX)) GOTO 18
18 NPX=NX-IND+1
RETURN
17 IF(XA<TAB(NX)) GOTO 17
16 IF(XA<TAB(NX)) GOTO 16
15 IF(XA<TAB(NX)) GOTO 15
14 IF(XA<TAB(NX)) GOTO 14
13 IF(XA<TAB(NX)) GOTO 13
12 IF(XA<TAB(NX)) GOTO 12
11 IF(XA<TAB(NX)) GOTO 11
10 IF(XA<TAB(NX)) GOTO 10
9 IF(XA<TAB(NX)) GOTO 9
8 IF(XA<TAB(NX)) GOTO 8
7 IF(XA<TAB(NX)) GOTO 7
6 IF(XA<TAB(NX)) GOTO 6
5 IF(XA<TAB(NX)) GOTO 5
4 IF(XA<TAB(NX)) GOTO 4
3 IF(XA<TAB(NX)) GOTO 3
2 IF(XA<TAB(NX)) GOTO 2
1 IF(XA<TAB(NX)) GOTO 1
0 IF(XA<TAB(NX)) GOTO 0
SUBROUTINE LAGRAN(XA,YA,SUM)
LAGRAN PERFORMS THE SUMMATION
DIMENSION X(1),Y(1)
SUM=0
DO 3 I=1,N
3 SUM=SUM+X(I)*Y(I)
RETURN
END
SUBROUTINE SIMPSON(XA,YA,DEL,IMAX,SUM,IER)
SIMPSON INTEGRATION ROUTINE.
END
IF (BA) 20,19,20
19 \text{IER} = 1\text{ RETURN}
20 \text{IF(DEL)} 22, 22, 23
22 \text{IER} = 2\text{ RETURN}
23 \text{IF(IMAX = 1)} 24, 24, 25
24 \text{IER} = 3\text{ RETURN}
25 X = BA/2, *A
00290 \text{NH} \text{HALF} = 1
00300 \text{SUMK} = (X) * BA * 2. / 3
00310 S = SUMK * (1.21) * (1.8) * BA/6,
00320 \text{DO 29 } I = 2, IMAX
00330 S1 = S
00340 S = S - SUMK / 2.1 / 2
00350 \text{NH} \text{HALF} = \text{NH} \text{HALF} + 2
00360 ANH\text{LF} = \text{NH} \text{HALF}
00370 FRST = A * 184/ANH\text{LF} / 2
00380 SUMK = (FRSTX)
00390 X = FRSTX
00400 KL\text{AST} = NHALF - 1
00410 FIX = BA * ANH\text{LF}
00420 \text{DO 29 } K = 1, KLAST
00430 X = FRSTX
00440 \text{SUMK} = \text{SUMK} * F(XK)
00450 \text{SUMK} = \text{SUMK} * 2. * BA / (3. * ANH\text{LF})
00460 S = S + SUMK
00470 \text{IF(S EQ 0.0)} \text{GO TO 29}
00480 \text{IF(ABS(S-S11)/ABS(S)) = DEL)} 29, 29, 29
00490 \text{CONTINUE}
00500 \text{IER} = 4
00510 \text{OUTPUT(108) IER, S11, S}
00520 \text{GO TO 30}
00530 \text{IER} = 0
00540 \text{GO TO 30}
00550 \text{N} = 2 * NHALF
00560 \text{RETURN}
00570 \text{END}