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

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Interim Report

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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 μm/s. A theoretical analysis of the measured axial compositional profiles was used to establish the liquid HgTe-CdTe interdiffusion 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.
PREFACE

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.
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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 µm/s. The temperature gradients at the solid-liquid interface, except for the 5.62 µm/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\cdot 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 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 99.99999% 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>
<thead>
<tr>
<th>Sample no.</th>
<th>Composition (x)</th>
<th>Quantity (moles)</th>
<th>Comments</th>
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<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>
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<td>0.06</td>
<td>A, C</td>
</tr>
<tr>
<td>5</td>
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<td>0.06</td>
<td>A, B, C</td>
</tr>
<tr>
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</tr>
<tr>
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<td>A</td>
</tr>
<tr>
<td>8</td>
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<td>0.06</td>
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</tr>
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<tr>
<td>11</td>
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<td>B</td>
</tr>
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<td>0.06</td>
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<tr>
<td>15</td>
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</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>Stoichiometric Te (g)</th>
<th>Excess Hg (mg)</th>
</tr>
</thead>
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<tr>
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<td>10.8345</td>
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</tr>
<tr>
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<td>1.3501</td>
<td>7.6570</td>
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<tr>
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<td>5.9</td>
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<tr>
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</tr>
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<td>7.2582</td>
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<td></td>
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<tr>
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<td>4.7582</td>
<td>7.7183</td>
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<tr>
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<td></td>
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</tr>
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<td>15.3200</td>
<td>2.4083</td>
<td></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 achieve 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 $T$.
$\frac{dT}{dt} = 2^\circ C/min$

Figure 5. Differential thermal analysis data for $Hg_{0.8}Cd_{0.2}Te$. 

Temperature ($^\circ C$)
Figure 6. DTA data for $x = 0.1, 0.2, 0.3, 0.4, 0.8, 0.7, 0.8$ and $0.9 \text{Hg}_x\text{Cd}_{1-x}\text{Te}$ alloys.
Considering radiation heat transfer only, the heat balance at the outer wall of the sample ampule yields

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

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

\[ T_s^4 = T^4 \left[ \left( 1 + \frac{r_q}{r_s} \right) \frac{\varepsilon_P}{\varepsilon_s} - \frac{r_q}{r_s} \frac{\varepsilon_F}{\varepsilon_s} \right] + 4S t^3 \left( 1 + \frac{r_q}{r_s} \right) \frac{\varepsilon_P}{\varepsilon_s} - 4P'T^3 \frac{r_q}{r_s} \frac{\varepsilon_F}{\varepsilon_s}. \]  

(4)

A first-order expansion in \( f/T \) and \( P'/T \) yields

\[ T_s = a_1 T + a_2 S - a_3 P', \]

(5)

where \( a_1, a_2, \) and \( a_3 \) are functions of \( r_q/r_s, \varepsilon_P/\varepsilon_s, \) and \( \varepsilon_F/\varepsilon_s. \)

For HgTe the observed empirical correlation between \( T, S, \) and \( T_s \) is given by

\[ T_s = T + 2S - P. \]

(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

\[ T_s = T - S_0 + 2S - P. \]

(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 \( 1.3^\circ C \) to \( 3.4^\circ C, \) which agree reasonably with finite-difference calculations that include both radiation and conduction heat transfer.

The solidus temperatures were determined by replotting 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.
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 of 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 10°C/at.% Te, and the Hg-Te liquidus temperature decreases at 1.2°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

$$P = P_0 \exp\left(21.732 - \frac{T_0}{T}\right),$$

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 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 $x = n_{\text{Cd}}/(n_{\text{Cd}} + n_{\text{Hg}})$. The phase diagram data are plotted in Figure 8.

**TABLE 4. FREE-VOLUME CORRECTION PARAMETERS AND CORRECTED LIQUIDUS TEMPERATURES.**

<table>
<thead>
<tr>
<th>Cd composition ($x$)</th>
<th>Capsule free volume (cm$^3$)</th>
<th>Te fraction (%)</th>
<th>Liquidus temperature correction ($^\circ$C)</th>
<th>Observed liquidus temperature ($^\circ$C)</th>
<th>Corrected liquidus temperature ($^\circ$C)</th>
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</thead>
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<tr>
<td>0.1</td>
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<td>50.02</td>
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<td>733</td>
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<td>954</td>
</tr>
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<td>0.87</td>
<td>50.20</td>
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</table>
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>
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<tr>
<td>0.1</td>
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<td>690</td>
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<td>0.2</td>
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<tr>
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<td>810</td>
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<td>954</td>
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<tr>
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<td>850</td>
<td>0.707</td>
<td>99</td>
</tr>
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<td>0.8</td>
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<tr>
<td>0.9</td>
<td>0.905</td>
<td>950</td>
<td>0.907</td>
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</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.¹²,¹⁶ 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>Composition (x)</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>---</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>

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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 $1^\circ C$ 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\textsuperscript{17} and Blair and Newham\textsuperscript{18} were derived from DTA measurements. Harman's\textsuperscript{19} data are from chemical analyses of first-to-freeze regions of molten alloy samples. Steininger's\textsuperscript{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, \( k(T) = x^S(T)/x^L(T) \), 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:

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

and
\[ x^L(T) = D_1 T^* + D_2 T^{*2} + D_3 T^{*3} + D_4 T^{*4}, \]  

(11)

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>
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<td>0.607640</td>
</tr>
<tr>
<td>2</td>
<td>0.086277</td>
<td>0.077209</td>
</tr>
<tr>
<td>3</td>
<td>1.200139</td>
<td>0.696767</td>
</tr>
<tr>
<td>4</td>
<td>-0.665231</td>
<td>-0.381683</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, $M_L(T) = \frac{x^S(T) - x_0}{x^S(T) - x^L(T)}$, 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\textsuperscript{1,2} were performed, and a set of R.A.S. parameters was obtained by simultaneously least-squares-fitting the binary\textsuperscript{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\textsuperscript{21} to describe mixtures whose behavior was found experimentally to have certain regularities, and the definition of the term is essentially empirical. Subsequently, Guggenheim\textsuperscript{22} 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\textsuperscript{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\textsubscript{1-x}Te\textsubscript{x} and Cd\textsubscript{1-x}Te\textsubscript{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,\textsuperscript{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\textsuperscript{2}:

\[
[1 - y] \exp \left[ \frac{H}{RT} y^2 \right] = \frac{x_{AC}}{x_{AC}^*} \\
\times \exp \left[ \frac{\Delta H_1 + w x_2 (1 - 2x_1) + (\alpha_1 x_1 + \sigma_2 x_2 - 0.5\alpha_1) (1 - 2x_3)}{RT} - \frac{\Delta S_1}{R} \right],
\]

(12)
and

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

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,

and

- \( W \) = 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

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

(14)
where

\[ x_{AC} = \frac{1 - (1 - 4(1 - x)x/(1 + \kappa))^{1/2}}{1 + [1 - 4(1 - x)x/(1 + \kappa)]^{1/2}}, \]

\[ x_\ast = x_{AC} \quad (x = 0.5), \]

and \( \kappa \) is given in terms of the temperature-independent equilibrium constant, \( K \), by

\[ \kappa = K \exp \left( \frac{-a}{2RT} \right) = \left( \frac{\beta^2}{1 - \beta^2} \right). \]

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

\[ a_A = x_A \gamma_A = x_A \exp \left[ \frac{x_A^2}{RT} \right] \]

and

\[ a_C = x_C \gamma_C = x_C \exp \left[ \frac{(1 - x)^2}{RT} \right], \]

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

\[ x_A = x_1 [1 + x_{AC}] - x_{AC}, \]

and

\[ x_C = x_3 [1 + x_{AC}] - x_{AC}. \]

For the pseudobinary cut, \( x_3 = 0.5 = x_1 + x_2 \), so that Equations (12) and (13) become

\[ (1 - y) \exp \left[ \frac{\omega}{RT} y^2 \right] = \frac{x_{AC}}{x_{AC}^\ast} \exp \left[ \frac{\Delta H_1 + \omega x_2(1 - 2x_1 - \Delta S_1)}{RT} \right] \]
and
\[
y \exp \left[ \frac{W}{RT} (1 - y \gamma) \right] = \frac{x_{BC}}{x_{BC}^*} \exp \left[ \frac{\Delta H_2 + \omega x_1 (1 - 2x_2)}{R} - \frac{\Delta S_2}{R} \right],
\]
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 \( x_{iC}^* (i = A, B) \) 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
\[
a_C = x_C \gamma_C = 0.5 \left[ 1 - x_{AC} - x_{BC} \right] \gamma_C,
\]
where \( \gamma_A^*, \gamma_B^*, \) and \( \gamma_C \) are the activity coefficients given by
\[
\gamma_A = \exp \left[ \frac{\omega x_2^2 + 0.25 \alpha_1 + (\omega + \alpha_1 - \alpha_2) (0.5 x_2)}{RT} \right],
\]
\[
\gamma_B = \exp \left[ \frac{\omega x_1^2 + 0.25 \alpha_2 + (\omega - \alpha_1 + \alpha_2) (0.5 x_1)}{RT} \right].
\]
3.2 Regular Associated Solution Parameters for the HgCdTe Alloy System

The R.A.S. parameters \( \alpha_1, \alpha_2, \kappa_1, \kappa_2, \omega, \) and \( W \) for the HgCdTe alloy system were determined by simultaneously least-squares-fitting the metal-rich segments of the binary liquidus curves\(^3\text{-}^6\) and the pseudobinary (Figure 8) phase diagram. To facilitate the computations, Equations (22) and (23) were rewritten in the following forms:

\[
T = \frac{\Delta H_1 + \omega x_2 (1 - 2x_1) - W y^2}{R \left[ \ln(1 - y) - \ln \frac{x_{AC}}{x_{AC}^*} \right] + \Delta S_1} = T_2
\] (33)

and

\[
T = \frac{\Delta H_2 + \omega x_1 (1 - 2x_2) - W (1 - y)^2}{R \left[ \ln y - \ln \frac{x_{BC}}{x_{BC}^*} \right] + \Delta S_2} = T_3
\] (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:

\[
S = \sum_i \left[ \left( \frac{T_{c1} - T_{e1}}{T_{c1} - T_{e1}} \right)^2 + \left( \frac{HgTe - HgTe}{T_{c1} - T_{e1}} \right)^2 \right. \\
+ \left. \left( \frac{T_{31} - T_{e1}}{T_{31} - T_{e1}} \right)^2 + \left( \frac{HgCdTe - HgCdTe}{T_{31} - T_{e1}} \right)^2 \right]
\] (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 $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ solutions.

### Table 8. R.A.S. Parameters and Thermodynamic Data for the $\text{Hg-Cd-Te}$ 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>$\Delta S_1 = 9.2$  s.u. $= 38.5$ J/mol K$^{(a)}$</td>
</tr>
<tr>
<td>$\alpha_1 = 953.0$ cal/mol $= 3.987$ kJ/mol</td>
<td>$\Delta S_2 = 8.9$ s.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>$T_{f_1} = 943$ K$^{(a)}$</td>
</tr>
<tr>
<td>$W = 836.0$ cal/mol $= 3.498$ kJ/mol</td>
<td>$T_{f_2} = 1365$ 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 $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$.

<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>0.258</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, the partial pressures of the components over the pseudobinary melt can be related to the activities by the expressions

\[ P_{Hg} = a_{Hg} P_{Hg}^0 \tag{36} \]
\[ P_{Cd} = a_{Cd} P_{Cd}^0 \tag{37} \]

and

\[ P_{Te2} = a_{Te}^2 P_{Te2}^0 \tag{38} \]

where \( P_{Hg}^0 \), \( P_{Cd}^0 \), and \( P_{Te2}^0 \) are the vapor pressures over the standard states and the respective activities \( a_{Hg} \), \( a_{Cd} \), and \( a_{Te} \) 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. 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 (x)</th>
<th>$a_{Hg}$</th>
<th>$a_{Cd}$</th>
<th>$a_{Te}$</th>
<th>$p^0$$_{Hg}$ (a)</th>
<th>$p^0$$_{Cd}$ (b)</th>
<th>$p^0$$_{Te2}$ (c)</th>
<th>$p_{Hg}$ (atm)</th>
<th>$p_{Cd}$ (atm)</th>
<th>$p_{Te2}$ (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>21.7 (21.4)</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>100.0</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>0.044</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>0.066</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 (70.0)</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>255.0</td>
<td>7.250</td>
<td>0.880</td>
<td>36.5 (72.0)</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>10.900</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 Stemmer's experimental results (Ref 7)

$P^0_{Hg}$, $P^0_{Cd}$, and $P^0_{Te2}$ represent the vapor pressures over the elemental melts

(a) $P^0_{Hg}$ was obtained from the equation: $\log_{10} P^0_{Hg}$ (atm) = $3080$ $T$/K which gives $P^0_{Hg}$ with an accuracy of better than 1% [S. Sugawara et al., Bull. Jap. Soc.Mech. Eng. 5, 711 (1962)].

(b) $P^0_{Cd}$ was obtained from the equation: $\log_{10} P^0_{Cd}$ (atm) = $5300$ $T$/K which gives $P^0_{Cd}$ with an accuracy of better than 0.5% [D.R. Stull and G.E. Sline, Thermodynamic Properties of the Elements, (Am. Chem. Soc., Washington, D.C. 1956)].

(c) $P^0_{Te2}$ was obtained from the equation: $\log_{10} P^0_{Te2}$ (atm) = $5960$ $T$/K [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 Hg$_{1-x}$Cd$_x$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
Figure 17. Bridgman crystal-growth furnace assembly.

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.

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

$$a_o = 0.646153 + (0.73671 x + 1.90501 x^2 - 0.69347 x^3)/1000,$$

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

$$a_o = \sqrt[3]{\frac{[4x M_{Cd} + 4(1-x) M_{Hg} + 4 M_{Te}]/\rho_m}{1/3}},$$

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

$$\rho_m = \frac{W_a \rho_w - W_w \rho_a}{W_a - W_w},$$

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 \( g/cm^3 \) in \( \rho_m \) leads to an uncertainty of about 0.001 in calculating \( x \). The uncertainty in \( \rho_m \) can be approximated by

\[
\Delta \rho_m = \frac{(\rho_m + \rho_w) \Delta W_a + \rho_m \Delta W_w - W_a \Delta \rho_w}{W_a - W_w},
\]

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 \( \Delta W_w \),

\[
\Delta \rho_m = \frac{\rho_m \Delta W_w}{W_a - W_w} = \frac{\rho_m^2 \Delta W_w}{W_a \rho_w} = \frac{\rho_m^2 \Delta W_w}{W_a}.
\]

The uncertainty in \( x, \Delta x \), is thus given by

\[
\Delta x = \frac{\Delta W_w \rho_m^2}{2 \cdot 2 \cdot W_a},
\]

where the density is in the units of \( g/cm^3 \). 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 \( \pm 0.0002 \) \( g \) is achieved. To do significantly better requires an inordinate amount of time.
The following expression, from Reference 25, was used to calculate the density of the water in which the sample is immersed:

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

In this expression, \(t_w\) is the water temperature in °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 °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°C for 1 h in air at 0.1 Pa \((1 \times 10^{-3} \text{ Torr})\) 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>
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<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>
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<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>
<tr>
<td>Sample number</td>
<td>Distance from tip (cm)</td>
<td>Mass density (g/cm³)</td>
<td>Average composition (X)</td>
</tr>
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<td>---------------</td>
<td>----------------------</td>
<td>----------------------</td>
<td>-------------------------</td>
</tr>
<tr>
<td>L41TP</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>
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<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>
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</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>
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<td>L41K</td>
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<tr>
<td>L44</td>
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</tr>
<tr>
<td>L45</td>
<td>7.45</td>
<td>7.6334</td>
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<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>
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<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>
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<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
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-off 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, 5, and 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

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

(47)

where \( C_s(\xi) \) is the solute (CdTe) concentration at a distance \( \xi \) along an ingot of length \( L \), \( C_o \) 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\(^8\) 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 $k = 1$ is given by

$$C_S(t) = C_0 \left\{ 1 + \text{erf} \left( \frac{1}{2} \left( \frac{Rt}{D} \right)^{1/2} \right) + (2k - 1)e^{-k(1-k)} \left( \frac{Rt}{D} \right) \right\} \times \text{erfc} \left( \frac{2k - 1}{2} \left( \frac{Rt}{D} \right)^{1/2} \right) \right\} . \quad (48)$$

For the final composition-transient, they obtained the expression

$$C_S(t) = C_0 \left\{ 1 + \sum_{n=1}^{\infty} \frac{(2n + 1)}{1 + k} \frac{(1 - k)}{(2 - k)} \cdots \frac{(n - k)}{(n + k)} \right\} \times e^{-n(n+1)} \left( \frac{R(L-t)}{D} \right) \right\} . \quad (49)$$

In the limit $Rt >> D$, 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 $Rt > D$ 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
genometry 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 $6.0 \times 10^{-5} \text{ cm}^2/\text{s}$ 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 $4.5 \times 10^{-5}$ cm²/s and included the variations in $k$ and $R$ along the growth axis.
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.
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 $6.0 \times 10^{-5}$ cm$^2$/s and constant $k, R$. 

Ingot L3 
$Hg_{1-x}Cd_xTe$ 
$x = 0.200$ 
$L = 17.3$ cm 
$R_0 = 0.597$ $\mu$m/s 
$k_0 = 3.63$ 

Distance along ingot (cm)
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 $k$, $R$. 

Calculated for $D = 6.0 \times 10^{-5}$ cm$^2$/s and constant $k$, $R$ 

Measured 

GPO7-0750-55
Figure 36. A comparison between the experimental data for ingot L6 and the calculated results for a diffusion coefficient of $4.5 \times 10^{-5}$ cm$^2$/s and constant $k$, $R$. 

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

Ingot: L6
$Hg_{1.4}Cd_{0.6}Te$
$x = 0.202$
$L = 18.1$ cm
$R_D = 0.31$ $\mu$m/s
$k_D = 3.63$
5. THEORETICAL MODELING OF CHARGE-CARRIER CONCENTRATIONS 
AND ELECTRON MOBILITIES

Theoretical models and computer programs specific to Hg$_{1-x}$Cd$_x$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$^9,10$ the Kane three-band model$^{11}$ is
used to describe the Hg$_{1-x}$Cd$_x$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$^{11}$

$$E^3 + (\Delta - E_g) E^2 - \left(\frac{\Delta E_g + P^2 k^2}{E_g}\right) E - \frac{2}{3} \Delta P^2 k^2 = 0,$$

where $E$ is the band energy in terms of the crystal momentum wave vector $k$, $\Delta$
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.$^{11}$ 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

$$\rho_i(E) = \frac{k^2}{\pi^2} \frac{dk}{dE} = \frac{1}{2\pi^2} \left(\frac{3}{2}\right)^{3/2} \frac{E_i^2}{P^2} \lambda_i \quad (i = c, lh),$$

(55)
where

\begin{align}
\lambda_c(\xi) &= \frac{3\left[28\xi^2 + \delta (3 - \delta)\xi + \frac{4}{3} (1 - \delta)\xi - \frac{2}{3}\right] \left[\xi(\xi - 1)(\xi + 1)\right]^{1/2}}{2\left(\frac{3}{2}\delta + 1\right)^{5/2}}, \\
\lambda_{\text{th}}(\xi) &= \frac{3\left[28\xi^3 - \delta (3 - \delta)\xi^2 + \frac{4}{3} (1 - \delta)\xi + \frac{2}{3}\right] \left[\xi(\xi + 1)(\xi - 1)\right]^{1/2}}{2\left(\frac{3}{2}\delta - 1\right)^{5/2}},
\end{align}

(56)

(57)

\xi = E/E_g \quad \text{(58)}

and

\delta = E_g / \Delta \quad \text{(59)}

The crystal momentum as a function of energy is

\begin{equation}
\mathbf{k} = \left(\frac{3}{2}\right)^{1/2} \frac{E_g}{p} \mathbf{s}(\xi),
\end{equation}

(60)

where

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

(61)

The conduction-band wave functions are given by

\begin{equation}
|\mathbf{k}, c, \pm \rangle = e^{i\mathbf{k} \cdot \mathbf{r}} \left[ a |\text{SA}_z \rangle \pm b |(X \mp iY) \alpha_{\pm} \rangle + c |Z \alpha_{\pm} \rangle \right].
\end{equation}

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

\[
a = \frac{[\xi (\delta \xi + 1) (\delta \xi + \frac{2}{3})]^{1/2}}{N}, \quad \text{(63)}
\]

\[
b = \sqrt{2} (\xi - 1)\frac{1}{3N} \quad \text{(64)}
\]

and

\[
c = (\xi - 1)\frac{1}{2} (\delta \xi + \frac{2}{3})/N, \quad \text{(65)}
\]

where

\[
N = \left[ \xi (\delta \xi + 1) (\delta \xi + \frac{2}{3}) + \frac{2}{9} (\xi - 1) + (\xi - 1) (\delta \xi + \frac{2}{3})^2 \right]^{1/2}. \quad \text{(66)}
\]

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

\[
E_{hh} = \frac{\hbar^2 k^2}{2m_v u_v}, \quad \text{(67)}
\]

where \( u_v \) 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,

\[
n_e - n_{lh} - n_{hh} = N_D - N_A, \quad \text{(68)}
\]

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, \( m_0 \) is the free electron mass, and \( \gamma = E/k_B T \).

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 \( N_D - N_A = 5.6 \times 10^{14} \) cm\(^{-3}\).
Figure 37. Theoretical and experimental conduction-electron concentration for Hg0.617Cd0.183Te.
TABLE 15. PARAMETERS FOR ELECTRON-MOBILITY AND CHARGE-CARRIER-CONCENTRATION CALCULATION FOR \( Hg_{1-x}Cd_xTe \) 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) \text{ 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>( E_0 = 11 \text{ eV (longitudinal mode)} )</td>
<td>(3)</td>
</tr>
<tr>
<td></td>
<td>( E_1 = 9.5 \text{ eV (transverse modes)} )</td>
<td>(4)</td>
</tr>
<tr>
<td></td>
<td>( E_2 = 3 \text{ eV} )</td>
<td></td>
</tr>
<tr>
<td>Longitudinal sound velocity(^{d})</td>
<td>( v_L = (2.52 + 0.54x) \times 10^5 \text{ cm/s} )</td>
<td></td>
</tr>
<tr>
<td>Transverse sound velocity(^{d})</td>
<td>( v_T = (1.60 + 0.27x) \times 10^5 \text{ cm/s} )</td>
<td></td>
</tr>
<tr>
<td>Hg mass</td>
<td>( m_{Hg} = 200.59 \text{ a.m.u.} )</td>
<td></td>
</tr>
<tr>
<td>Cd mass</td>
<td>( m_{Cd} = 112.4 \text{ a.m.u.} )</td>
<td></td>
</tr>
<tr>
<td>Te mass</td>
<td>( m_{Te} = 127.60 \text{ 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} T + (1.91 - 10^{-3} T) x] \text{ eV} )</td>
<td>(6)</td>
</tr>
<tr>
<td></td>
<td>( (0.135 \leq x \leq 0.203) )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( E_g = [-0.303 + 1.73x + 5.6 \times 10^{-4} (1 - 2x) T ) + 0.25x^4] \text{ eV (0.23 \leq x \leq 0.61, 10 K \leq T \leq 300 K)}</td>
<td>(7)</td>
</tr>
<tr>
<td></td>
<td>( E_g = [-0.25 \times 1.59 x + 5.233 \times 10^{-4} (1 - 2.08 x) T ) + 0.327x^3] \text{ eV (0.13 \leq x \leq 0.6, 20 K \leq T \leq 300 K)}</td>
<td>(8)</td>
</tr>
<tr>
<td>Momentum matrix element coupling conduction and</td>
<td></td>
<td></td>
</tr>
<tr>
<td>valence bands(^{e})</td>
<td>( P = 8.55x \times 10^{-4} \text{ eV cm} )</td>
<td></td>
</tr>
<tr>
<td>Transverse effective charges</td>
<td>( e_T/e^* = 2.96 )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( 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>(9)</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></td>
</tr>
<tr>
<td></td>
<td>( -0.951826x^3 )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \varepsilon_\infty = 15.1077 - 13.8823x + 9.88928x^2 )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( -3.67133x^3 )</td>
<td></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></td>
</tr>
<tr>
<td>CdTe TO phonon frequency</td>
<td>( \omega_{CdTe}^{TO} = (152 - 9x) \text{ cm}^{-1} )</td>
<td>(9)</td>
</tr>
</tbody>
</table>
(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) $\nu_I = c_{11}/\rho$, $\nu_T = c_{44}/\rho$, $\nu = (-2.3x + 8) \text{ g/cm}^3$ (This approximate equation was obtained using data from J. Blair and R. Newnham (101). The value of $c_{11}$ for HgTe (300 K) is 50.8 GPa (111), 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 (121), while the value for CdTe is 19.9 GPa (122). Assuming a linear variation for $c_{44}$ as a function of $x$, $c_{44} = (-0.60x + 20.5) \text{ GPa}$. 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 $\hbar^2/m_0^* = (2\hbar^2/3)(2E_g + 1/(E_g + \Delta))$, where $x = 0.204$ and values of $m_0^* = 4.66 \times 10^{-3} m_0$, $E_g = 51.7 \times 10^{-3}$ eV, and $\Delta = 0.96$ eV were used (14).
(f) These approximate equations were obtained using the referenced data.


* 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

$$f(k) = f_0 - kc'(E) f_0' \cos \psi,$$

where $f_0$ is the unperturbed distribution function and $f_0' = \frac{df_0}{dE}$. 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

$$J_x = \frac{e}{\hbar^2} \int_{E_g}^{\infty} k^2 c'(E) f_0' dE,$$

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

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

The sum, $\sum_i \left( \frac{\partial f}{\partial t} \right)_i$, 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,

$$\frac{\partial f(k)}{\partial t} = 0$$

(78)
The field term is given by

$$\sum_i \left( \frac{\partial f}{\partial t} \right)_i = -\left( \frac{\partial f}{\partial t} \right)_F, \quad (79)$$

The field term is given by

$$\left( \frac{\partial f}{\partial t} \right)_F = \frac{\varepsilon \mathbf{E}}{\hbar} f' \cos \psi, \quad (80)$$

where $\varepsilon$ is the applied electric field. The scattering term is given by

$$\sum_i \left( \frac{\partial f}{\partial t} \right)_i = -\frac{i}{\hbar \tau} \sum_i \int V_1(k, k') \left[ k'c'(E) - k'c'(E') \right] dk' \cos \psi, \quad (81)$$

where

$$V_1(k, k') = W_1(k', k) f_o(k') \left[ 1 - f_o(k) \right] = V_1(k', k). \quad (82)$$

$W_1(k', k)$ is the transition probability per unit time per unit volume and is given by

$$W_1(k', k) = \left| H_1(k', k) \right|^2 \left( \frac{1}{3} \right)^{3/2} \Omega \left( E_{k'} - E_k \pm E_S \right), \quad (83)$$

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 as modified by Howarth and Sondheimer and Ehrenreich. The perturbation function is expanded in a complete set of trial functions,

$$c'(E) = \sum_{n=0}^{\infty} c_n \phi_n(E), \quad (84)$$
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 $\mu_{\text{LO}}$, $\mu_{\text{ac}}$, $\mu_{\text{dis}}$, $\mu_{\text{eh}}$, and $\mu_{\text{if}}$ 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 $N_D = 7.6 \times 10^{14}$ cm\(^{-3}\) and an acceptor density of $2.0 \times 10^{14}$ 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, $e_c^*$, associated with relative displacements of atoms in a unit cell. The Callen effective charge is related to the Szigeti effective charge, $e_S^*$, and the total transverse charge, $e_T^*$, by the relations

\[
e_c^* = \left[ \frac{e_m + 2}{3 e_m} \right] e_S^* \tag{A1}\]

and

\[
e_S^* = \frac{e_T^*}{e_m}, \tag{A2}\]

where $e_m$ is the high-frequency dielectric constant. The interaction is assumed to be screened by the dielectric function given by

\[
\varepsilon(\omega_L, q) = \varepsilon_m + \frac{(k_e^F)^2 + (k_{th}^F)^2}{q^2}, \tag{A3}\]

where $\omega_L$ is the longitudinal-phonon frequency, $q$ is the phonon wave vector, and $k_e^F$ and $k_{th}^F$ are the electron and light-hole Fermi-Thomas momenta given by
(k_{FT}^e)^2 = \frac{2e^2}{\pi} \left( \frac{2\mu^* m_e}{\hbar^2} \right)^{3/2} \left( \frac{k_B T}{\beta} \right)^{1/2} \int_{\beta^{-1}}^{\infty} dy \lambda_c(y) \frac{e^{y-z}}{(e^{y-z} + 1)^2}

\text{and}

(k_{FT}^h)^2 = \frac{2e^2}{\pi} \left( \frac{2\mu^* m_e}{\hbar^2} \right)^{3/2} \left( \frac{k_B T}{\beta} \right)^{1/2} \int_{0}^{\infty} dy \lambda_h(y) \frac{e^{y+z}}{(e^{y+z} + 1)^2}, \quad \text{(A5)}

where

\[ \mu^* = 3\hbar^2 e^2 \left( 4m_e \right)^{-1}, \quad \text{(A6)} \]

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

\[ \left( \frac{\partial f^T}{\partial t} \right)_{\text{LO}} = \frac{-e^2 \mu^* m_e k_B T (F_1 + F_2)}{\hbar \omega_{LO} n \lambda c E \varepsilon^2} \mathcal{L} (c') f' \cos \psi, \quad \text{(A7)} \]

where

\[ F_i = \frac{4\pi N_i e^2}{M_i} \left( \bar{M_i} \right)^2 \quad (i = 1 = \text{HgTe}, \ i = 2 = \text{CdTe}), \quad \text{(A8)} \]

\( N_i \) is the number of unit cells of the \( i \)th type per unit volume, \( \bar{M}_i \) is the reduced mass of the \( i \)th unit cell, and

\[ \mathcal{L} (c') = \beta^{-1} \left[ \left( f_+/f_o \right) (n_p + 1) \left( c' R_+ - c' S_+ \right) + \left( f_-/f_o \right) n_p (c'_- R_- - c'_- S_-) \right], \quad \text{(A9)} \]

The subscripts (\( \pm \)) refer to the evaluation of the function at \( y \pm \theta \), where
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:

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

$$S_\pm(y, \theta) = F_\lambda(y) F_\lambda(y \pm \theta) s^2 (s_{\pm}^2 + s^2) \sum_{n=0}^{2} \rho_\pm^n(y, \theta) v_\pm^n (y, \theta),$$  \hspace{1cm} (A12)

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

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

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

$$\rho_0^\pm(y, \theta) = (a a_{\pm}^2 - b b_{\pm}^2 (b c_{\pm} + c b_{\pm})/\sqrt{2}]$$

$$+ \frac{1}{2} (b c_{\pm} + c b_{\pm})^2 + \frac{1}{4} (b b_{\pm})^2,$$  \hspace{1cm} (A16)

$$\rho_1^\pm(y, \theta) = 2a a_{\pm} (b_{1} b_{1\pm} + c_{1} c_{1\pm})$$  \hspace{1cm} (A17)
\[ p_2^\pm (y, \theta) = \frac{3}{4} (b_1 b_1^\pm)^2 + \frac{1}{2} (b_1 c_1^\pm + c_1 b_1^\pm)^2 + \frac{1}{\sqrt{2}} \]

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

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

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

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

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

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

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

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

\[ q_\pm = s_\pm^2 + s^2, \]
The symbols $a$, $b$, and $c$ have been defined in Section 5.1. In the above, $R_-$ and $S_-$ are zero for $y - 0 - \beta^{-1} < 0$.

### A.2 Acoustical Phonon (ac) Scattering Mechanism

The longitudinal and transverse acoustical-phonon/electron interactions are characterized by three deformation potentials: $k_o$ for the longitudinal mode and $k_1$ and $k_2$ for the transverse modes. The acoustical-phonon contribution to the Boltzmann equation is given by

\[ \left( \frac{\partial f(k)}{\partial t} \right)_{ac} = \frac{2k_B T}{\pi \hbar \rho_m v_L^2} \left( \frac{\mu' \rho_m}{v_L} k_o^2 \right) \frac{E_g \lambda_c s}{f_o' \cos \psi c'} \]  
\[ \times \left[ F_L + \left( \frac{v_L}{v_T} \right)^2 F_T \right] \]

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

\[ F_L = A_1^2 + \frac{2}{3} (A_1 A_2 + A_4) \quad \frac{1}{2} (2A_1 A_3 + A_2^2 - A_4) \]
\[ + \frac{4}{5} A_2 A_3 + \frac{1}{3} A_3^2 \]
and

\[ F_T = \left( \frac{E_1^2}{E_0^2} \right) \left( B_1 + \frac{2}{3} B_2 + \frac{1}{2} B_3 + \frac{2}{5} B_4 + \frac{1}{3} B_5 + B_6 \right), \]  

(A29)

where

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

(A30)

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

(A31)

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

(A32)

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

(A33)

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

(A34)

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

(A35)

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

\[ \left. - (b + c/\sqrt{2})^2 \right], \]  

(A36)

\[ B_4 = 2b^2 \left( b + c/\sqrt{2} \right) (b + \sqrt{2} c), \]  

(A37)
\[ B_5 = -b^2(b + \sqrt{2}c)^2, \]  
\[ B_6 = \frac{1}{2}\left[ b^2c^2 + \frac{1}{3}\left( c^2 - \frac{1}{2}b^2 \right)^2 \right]. \]  

A.3 Ionized Impurity (ii) Scattering Mechanism

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

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

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

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

\( \varepsilon_0 \) 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

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

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

\[ \phi_0 = \ln \left( \frac{g_0^2 + 4a^2}{g_0^2} \right) - 4a^2 / (g_0^2 + 4a^2), \quad (A44) \]

\[ \phi_1 = \frac{g_0^2 + a^2}{2a} \ln \left( \frac{g_0^2 + 4a^2}{g_0^2} \right) - \frac{4(g_0^2 + 3a^2)}{(g_0^2 + 4a^2)}, \quad (A45) \]

\[ \phi_2 = \frac{g_0^2}{2a^2} \left[ - \frac{4(g_0^2 + a^2)}{g_0^2} + \frac{(g_0^2 + 2a^2)}{2a^2} \right] \frac{g_0^2 (g_0^2 + 4a^2)}{g_0^2} \ln \left( \frac{g_0^2 + 4a^2}{g_0^2} \right) - \frac{2(g_0^2 + 2a^2)}{g_0^2} g_0^2 \left( g_0^2 + 4a^2 \right), \quad (A46) \]

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

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

\[ \pi_2 = \frac{3}{4} b^4 + \sqrt{2} b^3 c + c^4, \quad (A49) \]
with

$$\xi_0^2 = \frac{\hbar^2 \left[ (k_e^2)^2 + (k_h^F)^2 + (k_{hh}^F)^2 \right]}{2\mu^m_0 E g \varepsilon_0}.$$  
(A50)

A.4 Electron-Hole (eh) Scattering Mechanism

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

$$\left( \frac{\partial f(k)}{\partial t} \right)_{eh} = \frac{\pi n_{eh} e^4}{\hbar \varepsilon_0^2} \frac{c}{3} \phi_{eh} f_e^c \cos \psi c'(E),$$  
(A51)

where $\phi_{eh}$ is the same as $\phi_{il}$ for ionized defect scattering except that $\xi_0$ is replaced by $\xi_m$, i.e.,

$$\xi_m^2 = \frac{\hbar^2 \left[ (k_e^F)^2 + (k_h^F)^2 + (k_{hh}^F)^2 \right]}{2\mu^m_0 E g \varepsilon_0}.$$  
(A52)

A.5 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

$$\left( \frac{\partial f(k)}{\partial t} \right)_{dis.} = \frac{E_{dis.}}{\hbar \xi_0^2} \left( \mu^m_0 \right)^2 a c_{n_{dis.}} (1 - x) E^2_{dis.} \phi_{dis.} c' f^c \cos \psi,$$  
(A53)

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
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 $N_n n_n^2 E_n^2$, where $N_n$ is the density of neutral point-defects, $v_n$ 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

$$\sum_1^1 \frac{3f(k)}{3t} = -\frac{e^2 \mu_m k_B T (F_1 + F_2)}{h^2 \omega L \lambda c s E_g^2} \mathcal{P}(c') f' \cos \psi,$$  \hspace{1cm} (A55)

where

$$\mathcal{P}(c') = \mathcal{P}_{LO}(c') - \left\{ a_{ac} \lambda_c^2 s^2 \left[ F_L + \left( \frac{\nu_L}{\nu_T} \right)^2 F_T \right] + a_{ii} \frac{\lambda_c^2}{s^2} \phi_{ii} \right.$$ \hspace{1cm} (A56)

$$+ a_{eh} \frac{c}{s} \phi_{eh} + (a_{\text{dis.}} + a_n) \lambda_c^2 s^2 \phi_{\text{dis.}} \right\} c'(E),$$

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:

\[ \mathcal{H}(c') = \frac{2^{1/2} \beta^2 \omega_L^2 e_n^2}{\epsilon (\mu'm_0)^{3/2} (F_1 + F_2)} (k_BT)^{1/2} s^2 \beta^{3/2} \]  

(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,

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

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

$$J_x = \frac{4e^2 \omega_L (k_B T)^2}{3\pi^2 \hbar^2 (v_1 + F_2)} \left( \frac{F_{\ell 0}^2}{L_0^2} + \frac{[(\mathcal{L},\ell)]^2}{L_1} + \frac{[(\mathcal{L},\ell)]^2}{L_2} + \ldots \right),$$

where

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

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

$$F_{mn} = \int_{-1}^{\infty} \phi_m \mathcal{L}(\phi_n) \phi_o' \, dy,$$

and

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

$$\sigma = \frac{J}{E},$$  \hspace{1cm} (A70)

and the electron mobility is given by

$$\mu = \sigma / n_e.$$  \hspace{1cm} (A71)
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>VL = longitudinal sound velocity as a function of x.</td>
</tr>
<tr>
<td>01000</td>
<td>VT = 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>Line no.</td>
<td>Comments</td>
</tr>
<tr>
<td>----------</td>
<td>----------</td>
</tr>
<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} = ) LO phonon temperature.</td>
</tr>
<tr>
<td>01230</td>
<td>WL2 = longitudinal optical phonon frequency (CdTe), ( k_B \theta_{e2}/\hbar ), where ( \theta_{e2} = ) LO phonon temperature.</td>
</tr>
<tr>
<td>01240</td>
<td>EG = ( E_g ) (ergs) as a function of ( x ) and ( T ) (temperature).</td>
</tr>
<tr>
<td>01250</td>
<td>P = momentum matrix element coupling conduction and valence bands (eV-cm) as a function of ( x ).</td>
</tr>
<tr>
<td>01260</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>
</tbody>
</table>
| 01370   | CON = \[
\frac{2e^2}{\pi} \left( \frac{2\mu^* m_0}{\hbar^2} \right)^{3/2} \left( \frac{k_B T}{\beta} \right)^{1/2} \]
\( \text{i.e.,} \ (k_{FT}^e)^2, (k_{FT}^h)^2, \) and \( (k_{FT}^{hh})^2 \). |
<p>| 01780   | SIMP = an external program for evaluating integrals. |
| 01790   | KFTE2 = electron Fermi-Thomas momentum. |
| 01810   | KFTLH2 = light-hole Fermi-Thomas momentum. |
| 01820   | KFTHH2 = heavy-hole Fermi-Thomas momentum. |
| 01840   | THETA1 = ( \theta_{e1}/T ) (see line no. 01220). |
| 01850   | THETA2 = ( \theta_{e2}/T ) (see line no. 01230). |
| 01860   | GINF2 = ( g_{20}^2 ), a parameter involving Fermi-Thomas momenta. |
| 01870   | GO2 = ( g_{20}^2 ), a parameter involving Fermi-Thomas momenta. |
| 01890   | A1 = longitudinal optical (LO) phonon scattering contribution. |
| 01910   | A2 = acoustic phonon (ac) scattering contribution. |
| 01930   | A3 = ionized impurity (ii) scattering contribution. |
| 01950   | A4 = electron-hole (eh) scattering contribution. |
| 01960   | A5 = disorder scattering (dis.) contribution. |
| 01980   | NP1 = phonon occupation number. |
| 01990   | NP2 = phonon occupation number. |
| 02150   | Q1 = ( L_1 ) (matrix element). |
| 02160   | Q2 = ( J_2 ) (matrix element). |</p>
<table>
<thead>
<tr>
<th>Line no.</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>02170</td>
<td>$Q_3 = \mathcal{D}_3$ (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>$\varepsilon_{OPT} = k_B T / \beta$.</td>
</tr>
</tbody>
</table>
### B.2 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 ((E_1, E_2, E_3)) 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. 02710</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. 02780</td>
<td>SIMP - A subroutine used for evaluating a certain class of integrals.</td>
</tr>
<tr>
<td>B. 02800</td>
<td>NE = electron concentration.</td>
</tr>
<tr>
<td>B. 02800</td>
<td>NLH = light-hole concentration.</td>
</tr>
<tr>
<td>B. 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 \times LAMDA).</td>
</tr>
<tr>
<td>D. 03080</td>
<td>LAMDA - A function used to calculate the conduction band density-of-states.</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_{ch} \exp(y - z)/(\exp(y - z) + 1)^2).</td>
</tr>
<tr>
<td>E. 03080</td>
<td>LAMDA = (\lambda_c), an expression used in calculating the conduction-band density-of-states.</td>
</tr>
<tr>
<td>E. 03080</td>
<td>LAMDAV = (\lambda_{chs}), an expression used in calculating the light-hole density-of-states.</td>
</tr>
<tr>
<td>E. 03080</td>
<td>S - This program evaluates a function used in determining the crystal momentum.</td>
</tr>
<tr>
<td>L. 03080</td>
<td>L1 - This program evaluates (L^{(n)}).</td>
</tr>
<tr>
<td>N. 03080</td>
<td>NABC - This program evaluates the function (F_{\lambda}(y)), which appears in the LO-phonon scattering operator (\mathcal{G}_{LO}).</td>
</tr>
<tr>
<td>O. 04390</td>
<td>ROP1 = (\rho_0^+(y, \theta_1))</td>
</tr>
<tr>
<td>O. 04410</td>
<td>ROP2 = (\rho_0^+(y, \theta_2))</td>
</tr>
<tr>
<td>O. 04440</td>
<td>ROM1 = (\rho_0^-(y, \theta_1))</td>
</tr>
<tr>
<td>O. 04470</td>
<td>ROM2 = (\rho_0^-(y, \theta_2))</td>
</tr>
<tr>
<td>O. 04530</td>
<td>R1P1 = (\rho_1^+(y, \theta_1))</td>
</tr>
<tr>
<td>O. 04540</td>
<td>R2P1 = (\rho_2^+(y, \theta_1))</td>
</tr>
<tr>
<td>O. 04590</td>
<td>R1P2 = (\rho_1^+(y, \theta_2))</td>
</tr>
<tr>
<td>O. 04600</td>
<td>R2P2 = (\rho_2^+(y, \theta_2))</td>
</tr>
<tr>
<td>O. 04680</td>
<td>R1M1 = (\rho_1^-(y, \theta_1))</td>
</tr>
<tr>
<td>O. 04670</td>
<td>R2M1 = (\rho_2^-(y, \theta_1))</td>
</tr>
<tr>
<td>O. 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>$R_{2M2} = \mu_2^-(y, \theta_2)$</td>
</tr>
<tr>
<td>04760</td>
<td>$S_{Y2} = \sigma^2$</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>
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<tr>
<td>04840</td>
<td>$P_{1P} = P_1^+$</td>
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<td>04850</td>
<td>$P_{2P} = P_2^+$</td>
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<td>04870</td>
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<tr>
<td>04890</td>
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<tr>
<td>04910</td>
<td>$V_{1P} = r_1^+$</td>
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<tr>
<td>04920</td>
<td>$V_{2P} = r_2^+$</td>
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<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>$V_{0P1} = V_0^+(y, \theta_1)$</td>
</tr>
<tr>
<td>05010</td>
<td>$V_{1P1} = V_1^+(y, \theta_1)$</td>
</tr>
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<td>$V_{2P1} = V_2^+(y, \theta_1)$</td>
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<td>$V_{3P1} = V_3^+(y, \theta_1)$</td>
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<td>$V_{3P3} = V_3^+(y, \theta_2)$</td>
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<td>05190</td>
<td>$V_{0M1} = V_0^-(y, \theta_1)$</td>
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<td>$V_{2M1} = V_2^-(y, \theta_1)$</td>
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<td>05230</td>
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<td>$V_{0M2} = V_0^-(y, \theta_2)$</td>
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<td>$V_{2M2} = V_2^-(y, \theta_2)$</td>
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<tr>
<td>05330</td>
<td>$V_{3M2} = V_3^-(y, \theta_2)$</td>
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<tr>
<td>05390</td>
<td>$R_{P1} = R_+(y, \theta_1)$</td>
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<tr>
<td>05400</td>
<td>$S_{P1} = S_+(y, \theta_1)$</td>
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<tr>
<td>05430</td>
<td>$R_{P2} = R_+(y, \theta_2)$</td>
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<tr>
<td>05440</td>
<td>$S_{P2} = S_+(y, \theta_2)$</td>
</tr>
<tr>
<td>05480</td>
<td>$R_{M1} = R_-(y, \theta_1)$</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, θ_1)</td>
</tr>
<tr>
<td>05560</td>
<td>RM2 = R_−(y, θ_2)</td>
</tr>
<tr>
<td>05570</td>
<td>SM2 = S_−(v, θ_2)</td>
</tr>
<tr>
<td>05620</td>
<td>PI0 = π_0(y)</td>
</tr>
<tr>
<td>05640</td>
<td>PI2 = π_2(y)</td>
</tr>
<tr>
<td>05690</td>
<td>PHI0 = φ_0(y)</td>
</tr>
<tr>
<td>05710</td>
<td>PHI1 = φ_1(y)</td>
</tr>
<tr>
<td>05730</td>
<td>PHI2 = φ_2(y)</td>
</tr>
<tr>
<td>05770</td>
<td>PHI = Φ</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>056940</td>
<td>FLY = F_L(y)</td>
</tr>
<tr>
<td>05960</td>
<td>FTY = F_T(y)</td>
</tr>
<tr>
<td>103010</td>
<td>LB = L_B(y)</td>
</tr>
</tbody>
</table>

P.   ROOT - This program calculates limits.
Q.   INTEG - This program evaluates integrals.
R.   FMN - This program calculates the elements of the determinant F_{mn}(y).
S.   FM - This program evaluates a function involving FVP and L1.
T.   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 e_{o} and e_{∞}.

<table>
<thead>
<tr>
<th>Line No.</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<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 = e_{∞} as a function of x.</td>
</tr>
<tr>
<td>07550</td>
<td>EPS0 = e_{o} as a function of x.</td>
</tr>
</tbody>
</table>

GP02-0750-68
<table>
<thead>
<tr>
<th>Line No.</th>
<th>Comments</th>
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<tbody>
<tr>
<td>07560</td>
<td>WT2 = ωT (CdTe) as a function of x.</td>
</tr>
<tr>
<td>07570</td>
<td>WT1 = ωT (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>THL1 = HgTe LO - phonon temperature.</td>
</tr>
<tr>
<td>07782</td>
<td>THL2 = 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>
B.3 Computer Program Flow Charts

*FIXED
$SOURCE:CUBE.M0326B
$SOURCE:FFCTS.M0326B
$SOURCE:SIMP.M0326A

MERGE FFCTS. INTRPL. CUBE ? SIMP

REAL KFTE2,KFTLH2,KFTHH2
REAL M31(3,3),MJL(31)
LOGICAL GEND
REAL NE,NLM,NHH,NN1,NN2
REAL K,ND,KT,MO,MI,M2,MOD,NA
REAL ND1
REAL MB1,M2B
DIMENSION ISBSCP(7),VALUE(7),PARAM(7)

COMMON /NNN/ NE,NLM,NHH,ND1
COMMON /CONST1/ PX,PX,vX,MO.D,EY,FBC,YBC,YBV,NA,Z1,ZA
COMMON /VAR/ Z,CON
COMMON /NM/ N,M
COMMON /CONST2/ BETA,DDELTA,B

COMMON /CONST3/ THETA1,THETA2,GDF2,G02,EPHI0,EPHI1,EPHI2,
V1,V2,V3,V4,V5

COMMON /CONST4/ NF1,NP2,X1,X2,A1
EXTERNAL FUNC3,FUNC4
EXTERNAL FNM,FNM
WRITE(6,1)

FORMAT(13PARAMETER LIST/1 1 ** THINT/1 2 ** THAXT/1 3 ** T.
/DELTA/ 4 ** DONOR DENSITY/1 5 ** ACCEPTOR DENSITY/1
 6 ** PROPORTION OF CID IN ALLOY/1 7 ** DISORDER
ENERGY IN EV/1)

ES=4.80325E-10
MB=1.0545919E-27
K=1.3806522E-16
MO=9.1095558E-28
PI=3.141593
CEVE=1.821917E-12

CALL FFCTS

NRUN=1

CONT. ON PG 2
IF(NRUN.EQ.1) T
GO TO 21
WRITE(6,31)

3 I = 1,YES. 2=NO/
READ(2,1) NCONT

IF(NCONT.EQ.2) T
GO TO 550

21 NRUN=NRUN+1
WRITE(6,41)

FORMAT(ENTER NUMBER OF PARAMS TO BE CHANGED AND I.,
IPARM NO.,NEW VALUE) I/FOR EACH CHANGE///
READ(2,1) NCHNGE(1:BSCP(1).VALUE(1).I=1.NCHNGE)
DO 25 I=1,NCHNGE - - - D 3
J=ISBSCP(1)

CONT. ON PG 3
CON = CON*SQT(CN1/12.*PI*PI*SQT(BETA))
Z = 1000./T
DELZ = 0.3*Z
GEND = .FALSE.

70
XDL = FUNC(2)

IF XDL.LT.0.0)

T
GO TO 75

F

GEND = .TRUE.

XDU = XDL
Z = Z - DELZ
GO TO 70

75

IF (GEND)

T
GO TO 90

F
GO TO 85

80
XDL = XDU

CONT ON PG 6

PG 5 OF 10
SUBROUTINE SECULAR(KS,E1,E2,E3)

REAL KT,ND,MO,NA
REAL KS
COMMON /CONST/ PI,P,HB,KT,ND,UV,MO,D,EG,YBC,YBV,NA,Z1,ZA
C0=P*P*KS*KS
C2=0-EG
C1=-(EG*O+C0)
C0=+2.0*C0/3.

CALL CUBE(C2,C1,C0,E1,E2,E3)
RETURN
END

ORIGINAL PAGE IS
OF POOR QUALITY
FUNCTION FUNC1(X1)

REAL NE,NLH,NHH
REAL KT,ND,MO,NA
REAL NOD,ND1
COMM /CONST1/ PI,P,H,K,KT,ND,UV,MO,D,E,YBC,YBV,WA,ZI,ZA
COMM /NNN/ NE,NLH,NHH,ND1
COMM /VAR/ Z,CON
COMM /CONST2/ BETA,DELTA,BI
EXTERNAL FUNC1,FUNC2

NE=0.0
X2=10.+BI

IF(Z.GT.BI)

T
X2=10.+Z

X2=AMINI(YBC,X2)

IF(XZ.LE.BI)

T
GO TO 100

CALL SIMPLFUNC1, BI,X2,0.01,10.SI,NE,N.IER

NE=CONWNE

100
NLH=0.0

CONT. ON PG 2
\[ X_2 = 10. \]

\[ \text{IF}(Z \text{ LT} 0.0) \]

\[ X_2 = (10. - Z) \]

\[ X_2 = \text{AMIN}(YV, X2) \]

\[ \text{IF}(X2 \text{ LE} 0.0) \]

\[ \text{GO TO 200} \]

\[ \text{CALL SIMP}(\text{FUNC}, 0.0, X2, 0.0, 10, \text{SI}, \text{NLH}, \text{N}, \text{IER}) \]

\[ \text{NLH} = \text{CON} \times \text{NLH} \]

\[ \text{NHH} = (1.2 \times \text{UV} \times 10^{-9} \times \text{KT}) / (\text{HB} \times \text{HB}) \times (3.1 / 2.1) \]

\[ \text{NHH} = \text{NHH} \times (1. - 2) / (2. \times \text{PI} \times \text{PI}) \]

\[ \text{ED} = 0.003 \times 1.6921917 \times 10^{-12} \]

\[ E2 = E2 - E0 \]

\[ ND = 1.0 \times 10^{-5} \times (0.5 \times \text{EXP}(-E2 / \text{KT} + Z) + 1.0) \]

\[ NDI = ND \times NDD \]

\[ \text{FUNC} = \text{NE} - \text{NLH} - \text{NHH} - NDI \times Z1 + \text{NA} \times ZA \]

\[ \text{RETURN} \]

\[ \text{END} \]
FUNCTION FV(Y, Z)

IF(Y+Z .LE. 500.)

GO TO 10

IF(Y+Z .LE. 500.)

GO TO 20

FV = 0.0

GO TO 30

10

FV = 1.0

GO TO 30

20

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

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 FVP(Y,Z)

IF(Y+Z.LE.-200.)
  F
    T
    GO TO 10

IF(Y+Z.LE.-200.)
  F
    T
    GO TO 20
    FVP=0.0
    GO TO 30

10
  FVP=0.0
  GO TO 30

20
  FVP=EXP(Y+Z)
  FVP=FVP/(FVP+1.)/(FVP+1.)

30
  CONTINUE
  RETURN

END
FUNCTION FUNC3(Y)

REAL LAMDA
COMMON /VAR/ Z, CON
FUNC3=LAMDA(Y)*FVP(Y,-Z)
RETURN
END

FUNCTION FUNC4(Y)

REAL LAMDAV
COMMON /VAR/ Z, CON
FUNC4=LAMDAV(Y)*FVP(Y,Z)
RETURN
END
C

FUNCTION S(Y)

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

IF(Y.EQ.BI)
    F
    T
    BY = 1.

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

C

REAL FUNCTION LI(Y)

COMMON /CONST2/ BETA, DELTA, BI
LI = S(Y)/SQRT(BETA)
LI = LI*LI*LI
RETURN
END
FUNCTION H(Y,THETA)

H=0.0

IF (Y.LT.THETA)
T
RETURN

H=1.0
RETURN

END
SUBROUTINE NABC(Y, A, B, BP, C, CP, FL)

REAL N
COMMON /CONST2/ BETA, DELTA, BI
BY = BETA + Y

IF(Y.EQ.BI:
  N = SORT(Y*DBY + 1)*DBY23 + 2.*BY - 1. + (BY - 1.)*DBY23*DBY23)
  A = SORT(Y*DBY + 1)*DBY23/N
  B = SORT(2.*BY - 1.)*DBY23/N
  C = SORT(BY - 1.)*DBY23/N
  CP = SORT((3.*DBY/2. + 1.)/(BY*DBY + 1.))
  BP = SORT(2.*CP/(3.*N))
  DBY = DELTA*BI

FL = 3.*DBY*DBY*BY + DELTA*(3.*DBY/2.*BY + 1. - DELTA)
   *DBY/3. - 2./3.)/(2.*DBY/2.*BY + 1.*DBY/2.*BY + 1.)

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,
VLT,VT,SR2,SR3,SR4,SR5

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

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

SM1=S(Y-THETA1)

10

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

SM2=S(Y-THETA2)

CONT. ON PG 2

PG 1 OF 11
CALL NABC(Y, A, B, BP, C, CP, FL)

CALL NABC(Y + THETA1, AP1, BP1, BP1, CP1, CPP1, FLP1)

CALL NABC(Y + THETA2, AP2, BP2, BP2, CP2, CPP2, FLP2)

IF(YM18 .LT. 0.0)

T

GO TO 30

CALL NABC(Y - THETA1, AM1, BM1, BPM1, CM1, CPM1, FLM1)

30

IF(YM28 .LT. 0.0)

F

T

GO TO 40

CALL NABC(Y - THETA2, AM2, BM2, BPM2, CM2, CPM2, FLM2)

40

CONTINUE

S2 = SORT(2.1)
BC = B * CP2 + C * BP2
BC = B * CP2 + C * BP2

CONT. ON PG 3
IF(M1B.LT.0.0)
  T
  GO TO 70
  BB=BP*BPM1+CP*CPM1
  BC=BP*CPM1+CP*BPM1
  BX=BP*BPM1
  CX=CP*CPM1
  R1M1=2.*RA*AM1*BB
  R2M1=3.*B*BX/4.*B*BC/S2+2.*BX*CX-BC*BC/2.+CX*CX

70
  IF(M2B.LT.0.0)
  T
  GO TO 80
  BB=BP*BPM2+CP*CPM2
  BC=BP*CPM2+CP*BPM2
  BX=BP*BPM2
  CX=CP*CPM2
  R1M2=2.*RA*AM2*BB
  R2M2=3.*B*BX/4.*B*BC/S2+2.*BX*CX-BC*BC/2.+CX*CX

80
  CONTINUE
  SY2=SY*SY
  01P=SP1*SP1+SY2
  02P=SP2*SP2+SY2

CONT. ON PG 5
PG 4 OF 11

124
S  A2

S  A3

110

IF(Y2B.LT.0.0)

T

GO TO 120

P2M=2RM+GINF2

120

CONTINUE

V1P=3Y*SP1
V2P=5T*SP2

IF(Y1B.LT.0.0)

T

GO TO 130

Y1M=SYM1

130

IF(Y2B.LT.0.0)

F 7

T 11

CONT. ON PG 7
\[ V_{2M1} = (1 - 2.471081)(1 - P_{1M}/Q_{1M}) \times P_{1M}/P_{1H}/P_{V1} + P_{1M}/(2.471081)(1 - \frac{P_{1M}}{Q_{1M}}) \times 1/4 \]

\[ V_{3M1} = -\frac{1}{16}(2.471081)(1 - P_{1M}/Q_{1M}) \times P_{1M}/P_{1H}/P_{V1} - \frac{1}{16}(2.471081)(1 - \frac{P_{1M}}{Q_{1M}}) \times 1/4 \]

\[ S_{P1} = R_{P1}/S_{Y2} \]
\[ R_{P1} = R_{P1}/S_{Y2} \]
\[ S_{P1} = S_{P1}/S_{Y2} \]
\[ R_{P2} = R_{P2}/S_{Y2} \]
\[ S_{P2} = S_{P2}/S_{Y2} \]

GO TO 16D

CONTINUE

CONT. ON PG 9

PG 80F 11
SUBROUTINE ROOT(F,A,B,TOL)

C

Z=1.0
FA=F(A)

IF(FA.GT.0.0)

T

Z=-1.0

A1

2

X=(A+B1/2.0)

Y=F(X)

IF(Y*X) 10,100,20

0

10

A=X

GO TO 30

20

B=X

CONT. ON PG 2

PG 10F 2
IF (B - A) LT TOL

RETURN

GO TO 7

RETURN

END
FUNCTION FM(Y)

REAL LI
COMMON VAR Z, CON
COMMON NM N, M
COMMON CONST2 BETA, DELTA, BI
X = Y - BI
XM = 0.0

IF(X.EQ.0.0)

T

GO TO 10

XM = XM

10 CONTINUE

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

RETURN

END
SUBROUTINE HCSPOLE(X, THT1, THT2, TML1, TML2, ESTP1, ESTR2, EPSO, EPS1, EC1, EC2)

ESTR = 2.96
ESTR2 = 2.35
XM1 = -.29500E-22
XM2 = 9.9239E-23
A = 6.46040 21X1.0E-8
PSO = 20.286 - 15.1531 X - 6.59091 X - 0.961328 X
WT2 = 52.0 - 9.0 X

WT1 = 118.0 + 12.0 X
ES = 4.88325E-10
HB = 1.0545919E-27
B2 = 1.388622E-16
P1 = 3.141593
C = 2.997925E10
THT1 = 2. X17 A X H B / B K W T1
THT2 = 2. X17 A X H B / B K W T2

OMT1 = B K * THT1 / H B
OMT2 = B K * THT2 / H B
S = F1 / O M T 1 X 2.
S2 = F2 / O M T 2 X 2.

TML2 = 1. / 2. * EPS1 X E PS1 X ( THT1 X 2 + THT2 X 2 ) + S1 * THT1 X 2.
+ S2 * THT2 X 2 + SORT (( EPS1 X ( THT2 X 2 - THT1 X 2 ) + S1 * THT1 X 2.
+ S2 * THT2 X 2)

THL2 = SORT (( EPS1 + S1) / EPS 1 * TH1
THL12 = TML2
THL22 = THL2

IF (THT2 .GT. THLD) THEN
T
GO TO 10
A1
TML12 = THL2

CONT. ON PG 2

PG 1 OF 2
\[ \begin{align*} 
\text{THL}_Z &= \text{SORT} \left( \text{THL}_1, \text{THL}_2 \right) \\
\text{THL}_1 &= \text{THL}_1 \quad \text{THL}_2 = \text{THL}_1 / 2 \\
\text{THL}_Z &= \text{ECI} / \text{EPSI} \\
\text{RETURN} \\
\text{END} \\
\end{align*} \]

ORIGINAL PAGE IS OF POOR QUALITY
01108 FIXED
01205 SOURCE FFCTS, M03268
01305 SOURCE SIMP, M03268
01405 COMMON FFCTS, SIMP, M03268
01505 REAL KJL, KJLH, KJLHM2, KJLHMH2
01605 REAL KM(3,3), ML(1,3)
01705 LOGICAL GENO
01805 REAL NE, NL=NH1, NP1, NPZ
01905 REAL KD, KT, M0, M2, M00, NA
02005 REAL NE, M0, NA
02105 DIMENSION ISBSCP(7), VALUE(7), PARM(7)
02205 COMMON /NNV/ NE, NL=NH1, NDI
02305 COMMON /CONST/ P1, P2, H6, KT, NDI, UV, M0, D, EG, YBC, YBV, NA, Z1, ZA
02405 COMMON /VAR/ Z, CON
02505 COMMON /M/ N, M
02605 COMMON /CONST/ NPI, NP2, X1, X2, A1
02705 COMMON /FUN3/ FUNC
02805 COMMON /FUN4/ Func
02905 REAL NP, NCHNGE(I)
03005 REAL K = L (6.5)
03105 REAL (6.6)
OF POOR QUALITY

FUNCTION FV(Y,Z)

02690 X2=AMIN1(YBC,X2)
02690 IF (X2.LT.0.0) GO TO 100
02710 CALL SIMP(FUNC1,Y,X2,0.01,10,S11,NE,N,N,E1R)
02710 NE=CUM*NE
02720 100 NLH=0.0
02730 IF (L1.LT.0.0) X2=(10.0-Z)
02750 X2=AMIN1(YBV,X2)
02770 IF (X2.LE.0.0) GO TO 200
02770 CALL SIMP(FUNC2,0.0,X2,0.01,10,S11,NLH,N,NE,N,E1R)
02780 NLH=CON*NLH
02790 200 NLH=(3.*FCV+1.5)*CNK/(HNH*N)*10.0
02800 ED=0.003*1.602197E-12
02802 E2=ED+0.0
02803 NDD=l.0*ED/(0.5*EXP(-E2/KT+2)*1.0)
02804 NU=ND*NU
02810 FUNCNE=NLH-NHH-ND1*Z1+NA*ZA
02820 RETURN
02830 END

FUNCTION FUNC1(Y)

02840 C

02850 FUNCTION FV(Y,Z)

02870 IF (Y.Z.LE.500.0) GO TO 10
02890 FV=0.0
02890 IF (Y.Z.LE.500.0) GO TO 20
02890 RETURN
02890 10 FV=1.0
02890 IF (Y.Z.LE.100.0) GO TO 30
02890 IF (Y.Z.LE.100.0) GO TO 20
02890 RETURN
02890 END

FUNCTION FUNC2(Y)

02900 REAL LAMDA
02902 COMMON /VAR/ Z,CON
02904 FUNC1=FV(Y-Z)*LAMDA(Y)
02906 RETURN
02906 END

FUNCTION FVP(Y,Z)

02910 IF (Y.Z.LE.200.0) GO TO 10
02910 IF (Y.Z.LE.200.0) GO TO 20
02910 FVP=0.0
02910 IF (Y.Z.LE.100.0) GO TO 30
02910 RETURN
02910 END

FUNCTION FVP(Y,Z)

02920 FUNCTION FUNC3(Y)

02930 REAL LAMDA
02932 COMMON /VAR/ Z,CON
02934 FUNC3=LAMDA(Y)*FVP(Y-Z)
02936 RETURN
02936 END

FUNCTION FVP(Y,Z)

02940 FUNCTION FUNC4(Y)

02950 REAL LAMDA
02952 COMMON /VAR/ Z,CON
02954 FUNC4=LAMDA(Y)*FVP(Y,Z)
02956 RETURN
02956 END

REAL FUNCTION LAMDA(Y)

02960 COMMON /CONST2/ BETA,DELTA,B1
02970 B1=BLTA+B1

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```
ORIGINAL PAGE IS OF POOR QUALITY

<table>
<thead>
<tr>
<th>Statement</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q3480 IF (Y_EQ_B) BY1</td>
<td></td>
</tr>
<tr>
<td>Q3490 LAMDA=2.<em>DELTA+DELTA</em>BY<em>BY+DELTA</em>(3.-DELTA)<em>BY</em>BY</td>
<td></td>
</tr>
<tr>
<td>Q3500 x=1.<em>DELTA</em>BY/2./2.</td>
<td></td>
</tr>
<tr>
<td>Q3510 LAMDA=3.2LAMDA<em>SQRT(BY</em>(BY+1.))<em>(DELTA-BY)+1.)/(X</em>X<em>X</em>X)/2.</td>
<td></td>
</tr>
<tr>
<td>Q3520 RETURN</td>
<td></td>
</tr>
<tr>
<td>Q3530 END</td>
<td></td>
</tr>
<tr>
<td>Q3540</td>
<td></td>
</tr>
<tr>
<td>Q3550 REAL FUNCTION LAMBDA(Y)</td>
<td></td>
</tr>
<tr>
<td>Q3560 COMMON /CONST2/ BETA+DELTA+BI</td>
<td></td>
</tr>
<tr>
<td>Q3570 RETURN</td>
<td></td>
</tr>
<tr>
<td>Q3580 IF (Y_EQ_B) BY1</td>
<td></td>
</tr>
<tr>
<td>Q3590 RETURN</td>
<td></td>
</tr>
<tr>
<td>Q3600 REAL FUNCTION L1(Y)</td>
<td></td>
</tr>
<tr>
<td>Q3610 COMMON /CONST2/ BETA+DELTA+BI</td>
<td></td>
</tr>
<tr>
<td>Q3620 RETURN</td>
<td></td>
</tr>
<tr>
<td>Q3630 IF (Y_EQ_B) BY1</td>
<td></td>
</tr>
<tr>
<td>Q3640 RETURN</td>
<td></td>
</tr>
<tr>
<td>Q3650 FUNCTION M(Y,THETA)</td>
<td></td>
</tr>
<tr>
<td>Q3660 COMMON /CONST2/ BETA+DELTA+BI</td>
<td></td>
</tr>
<tr>
<td>Q3670 RETURN</td>
<td></td>
</tr>
<tr>
<td>Q3680 IF (Y_EQ_B) BY1</td>
<td></td>
</tr>
<tr>
<td>Q3690 RETURN</td>
<td></td>
</tr>
<tr>
<td>Q3700</td>
<td></td>
</tr>
<tr>
<td>Q3710 CALL NABC(Y,RP1,RP2,RM1,RP2,SM1,SM2,BL)</td>
<td></td>
</tr>
<tr>
<td>Q3720</td>
<td></td>
</tr>
<tr>
<td>Q3730 CALL RSL1(Y,RP1,RP2,RM1,RP2,SM1,SM2,BL)</td>
<td></td>
</tr>
</tbody>
</table>
```

GO TO 30

IF YH < 0 THEN
   CALL NABC
   CONTINUE

BC = b * CM^2 * CYRM^2
RO = A^2 * A^2 * AM^2 - B * BM * BC - (BC^2) * BC / 2 * B * B * MZ / 4E

CONTINUE

SY^2 = 5r^2 / 5y
OLP = bP_1 * sP
;r = SY^2 + SY^2

IF YH < T.O THEN
   PM = Q * G
   CONTINUE

ULP = SY^2 + PI

CONTINUE

PI = OLP * G
NF2
PZP = ~P * CINFL
IF YH < T.O THEN
   PM = Q * G
   CONTINUE

OCH: U = INF
SUBROUTINE ROOT(F, A, B, TOL)

FA = F(A)
Y = FA + TOL
X = (A + B) / 2.
YF(X) = Y
Y = 100 * TOL
RETURN
END

SUBROUTINE INTEGRATION(F, R, A, B, YU)

FUNCTION FMN(Y)

REAL LRNP1, NPE

COMMON /VAR/ ZCON

COMMON /NM/ NNI, NMM

COMMON /CONST1/ BETA, DELTA, BI

COMMUN /CONST2/ THETA1, THETA2, GINF2, G02, EPHII, EPHII, EPHII2

1

COMMON /CONST3/ RNP1, RNP2, X1, X2, X11

REAL X, Y

FMN = Y

RETURN
END
FUNCTION FM(Y)

REAL X, Y, Z

COMMON /VAR/Z, CON
COMMON /NM/ N

COMMON /CONST2/ BETA, DELTA, BI

RETURN
END

SUBROUTINE CUBE(B, C, N, E1, E2, E3)

CUBE WRITTEN 9/19/74

JMP

COMMENTS:

THIS ROUTINE SOLVES THE GENERAL CUBIC EQUATION

X**3 + B*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, S0, Y, Z, S

C = CMPLX(-B, 0.0)

P = (B*B/3.0)**0.5

Q = (2.0*B*B/27.0) + (C*B/3.0)**0.5

F = (Q - P**2)**0.5

S = SQRT(F)

Y = 0.0

IF (CABS(S), NE, 0.0) Y = CEXP(CLOG(S)/3.0)
SUBROUTINE INTRPL(X,TABX,TABY,NC,YN,IND)
5 CONTINUE
30 IF (X.GT.20.) GO TO 20
300 X=0.0
3301 EXPX=EXP(A)
3302 F=CON(1+IK)*EXPX*(1-EXPX/CON(2+IK))
3303 RETURN
3304 CALL INTRPL(X*ETATAB,FT12(1),17+241,F,IND)
3305 IF (IND.EQ.0) RETURN
3306 WRITE(6,999)K,X
3307 CALL EXIT
3308 RETURN
3309 X=K/(X*2-1/2)
3310 RETURN
3311 END
3312 FUNCTION F(K2+ETA)
3313 DIMENSION CON(4,S)
3314 COMMON ETATAB(241),FTM12(241),FT12(241),FT32(241),FT52(241)
3315 IF (X.GE.10) GOTO 10
3316 X=ETA
3317 IF (X*LE.E+00.) GO TO 5
3318 EXPX=EXP(A)
3319 IF (X*LE.-200.) GO TO 5
3320 F=CON(1+IK)*EXPX*(1-EXPX/CON(2+IK))
3321 RETURN
3322 IF (X*,GT.20.) GO TO 20
3323 CALL INTRPL(X*ETATAB,FT12(1),17+241,F,IND)
3324 IF (IND.EQ.0) RETURN
3325 WRITE(6,999)K,X
3326 CALL EXIT
3327 RETURN
3328 X=K/(X*2-1/2)
3329 RETURN
3330 END
3331 COMMON ETATAB(241),FTM12(241),FT12(241),FT32(241),FT52(241)
3332 DATA CON/0.7725439,1.4121361,-41.2335,1.7756666,
3333 /1.8522593,2.824427,1.2335005,1.0556199,
3334 /0.6540905,0.5586542,0.180827,1.7756666,
3335 /1.32351,1.313708,1.39317,1.2429086,
3336 /1.63725,2.62717,2.5,907711,1.11168625/}

SUBROUTINE INTRPL(X,TABX,TABY,NC,YN,IND)
5 CONTINUE
30 IF (X.GT.20.) GO TO 20
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3301 EXPX=EXP(A)
3302 F=CON(1+IK)*EXPX*(1-EXPX/CON(2+IK))
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3318 EXPX=EXP(A)
3319 IF (X*LE.-200.) GO TO 5
3320 F=CON(1+IK)*EXPX*(1-EXPX/CON(2+IK))
3321 RETURN
3322 IF (X*,GT.20.) GO TO 20
3323 CALL INTRPL(X*ETATAB,FT12(1),17+241,F,IND)
3324 IF (IND.EQ.0) RETURN
3325 WRITE(6,999)K,X
3326 CALL EXIT
3327 RETURN
3328 X=K/(X*2-1/2)
3329 RETURN
3330 END
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3321 RETURN
3322 IF (X*,GT.20.) GO TO 20
3323 CALL INTRPL(X*ETATAB,FT12(1),17+241,F,IND)
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3330 END
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3333 /1.8522593,2.824427,1.2335005,1.0556199,
3334 /0.6540905,0.5586542,0.180827,1.7756666,
3335 /1.32351,1.313708,1.39317,1.2429086,
3336 /1.63725,2.62717,2.5,907711,1.11168625/}
SUBROUTINE LAGRAN(XA, YA, X, Y, SUM)
     DIMENSION X(1), Y(1)
     ONUM = 0
     ONUM = 1
     DUM = 3
     SUM = 0
     DUM = 0
     IF (A) THEN
         SUM = SUM + PROD
         DUM = DUM + 1
     END IF
     RETURN
END SUBROUTINE LAGRAN

SUBROUTINE SIMPSON(F, A, B, DEL, IMA, S1, S2, N, IER)

IF (A) THEN
    B = A
    S1 = 0
    S2 = 0
    IF (B) THEN
        S1 = S1 + F
        S2 = S2 + F
    END IF
    N = 1
END IF

IF (N) THEN
    S1 = S1 + F
    S2 = S2 + F
    N = N + 1
END IF

IF (N) THEN
    S1 = S1 + F
    S2 = S2 + F
    N = N + 1
END IF

IF (N) THEN
    S1 = S1 + F
    S2 = S2 + F
    N = N + 1
END IF

RETURN
END SUBROUTINE SIMPSON

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19 IER = 1
20 IF (DEL) 22, 22, 23
22 IER = 2
23 IF (IMAX = 1) 24, 24, 25
24 IER = 3
25 RETURN
26 X = 8A/2 + A
27 SUMK = (X) * BA/2 / 3
28 DO 29 I = 2, IMAX
29 SUMK = SUMK / 2
30 S = S - SUMK / 2 + 2
31 SUMK = SUMK / 2
32 NHALF = NHALF * 2
33 ANHALF = NHALF
34 S = S - SUMK / 2 + 2
35 SUMK = SUMK / 2
36 DO 29 K = 1, KLAST
37 X = X + FINC
38 SUMK = SUMK + F(XK)
39 SUMK = SUMK / 2 + BA / (3 * ANHALF)
40 IF (S = 0) GO TO 29
41 SUMK = SUMK / 2
42 IF (ABS(S - S11) / ABS(S)) = DEL) 29, 29, 29
43 CONTINUE
44 IER = 4
45 OUTPUT (108) IER, S1, S
46 GO TO 30
47 IER = 0
48 CONTINUE
49 N = 2 * NHALF
50 RETURN