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DEFECT CHEMISTRY AND CHARACTERIZATION OF $Hg_{1-x}Cd_xTe$

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George C. Marshall Space Flight Center

Alabama 35812

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HONEYWELL
Electro-Optics Operations
2 Forbes Road
Lexington, MA 02173

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DOPING BEHAVIOR OF IODINE IN $Hg_{0.8}Cd_{0.2}Te$[†]

H.R. Vydyanath and J.C. Donovan
HONEYWELL
Electro-Optics Operations
2 Forbes Road
Lexington, Massachusetts 02173

ABSTRACT

Iodine doped single crystal samples of $Hg_{0.8}Cd_{0.2}Te$ were annealed at temperatures varying from 450 to 600°C in Hg vapor and quenched to room temperature. Hall effect measurements at 77 K on the crystals cooled to room temperature indicate the samples to be n-type after anneals at high Hg pressures whereas they turn p-type after anneals at low Hg pressures; the electron concentration increases with increase in Hg pressure. The results are explained on the basis that the crystals are saturated with $(Hg,Cd)I_2$, with a fraction of the iodine being present as donors occupying tellurium lattice sites ($I_{Te}^{\bullet}$) and a fraction being present as acceptors $(I_{Te}V_{Hg})'$ resulting from the iodine on tellurium lattice sites ($I_{Te}^{\bullet}$) pairing with the doubly ionized native acceptor defects (V_{Hg}''). The solubility of the donor species increases with increase in Hg pressure, whereas that of the acceptor species increases with decrease in Hg pressure. Equilibrium constants for the incorporation of the iodine species as well as the pairing reaction have been established.

[†] This work was supported by NASA under contract NAS8-33245.

I. FOREWORD

This semiannual technical report covers the work performed by Honeywell Electro-Optics Operations, Lexington, Massachusetts from July 1, 1980 to December 31, 1980 under the NASA sponsored program entitled 'Defect Chemistry and Characterization of (Hg,Cd)Te' on Contract NAS8-33245. The objective of this program is to study and formalize the defect chemistry of (Hg,Cd)Te and to evaluate and select characterization methods for the material.

The principal investigator is Dr. H.R. Vydyanath providing the overall technical direction for the program. Assistance with the experimental work is provided by J.C. Donovan, P. Crickard and A. Barnes. R.A. Lancaster and D.A. Nelson generously furnished all the crystals required for the program.

II. INTRODUCTION

At the end of the first eighteen month period of the program the defect structures of undoped $Hg_{0.8}Cd_{0.2}Te$ (S), undoped $Hg_{0.6}Cd_{0.4}Te$ (S) copper and indium doped $Hg_{0.8}Cd_{0.2}Te$ (S) were established. These results were reported in the semiannual technical report covering the period of January 1979 to June 1980. This semiannual report details the work performed from July 1, 1980 to December 31, 1980. During this six month period, the defect structures of both phosphorous doped and iodine doped $Hg_{0.8}Cd_{0.2}Te$ have been investigated. The investigation of the phosporous doped crystals is still in programs whereas that of the iodine doped crystals is completed and will be described in this report. Iodine doped single crystal samples of $Hg_{0.8}Cd_{0.2}Te$ were annealed at temperatures ranging from 450 to 600°C in Hg vapor and were quenched to room temperature. Hall effect measurements at 77 K on these samples indicate the samples to be n type after anneals at high Hg pressures, whereas, they turn p type after anneals at low Hg pressures. The electron concentration increases with increase in the partial pressure of Hg. The results are explained on the basis that the crystals are saturated with (Hg,Cd) I_2, with a fraction of the iodine being present as donors occupying tellurium lattice sites ($I_{Te}^{\bullet}$) and a fraction being present as acceptors ($(I_{Te}V_{Hg})'$) resulting from the iodine on tellurium sites ($I_{Te}^{\bullet}$) pairing with the doubly ionized nature acceptor defect species (V''_{Hg}). The solubility of the donor species increases with increase in the partial pressure of Hg, whereas that of the acceptor species increases with decrease in Hg pressure. Equilibrium constants for the incorporation of the iodine species as well as for the pairing reaction have been established.

The following presentations and publications have resulted from the work performed from January 1, 1979 to December 31, 1980.

(1) '$(Hg_{1-x}Cd_x)Te$ Material Studies' H.R. Vydyanath, D.A. Nelson, R.A. Lancaster and R.G. Roy in proceedings of the IRIS Detector Specialty Group meeting, Minneapolis, MN June 15-17, 1979 p. 29.

(2) 'Defect Chemistry and Characterization of $(Hg_{1-x}Cd_x)Te$' H.R. Vydyanath, D.A. Nelson and R.A. Lancaster, Journal of Electrochem. Soc. 126, 371C (1979)

(3) 'Defect Studies in $Hg_{0.8}Cd_{0.2}Te$' H.R. Vydyanath, presented at the conference on the "Crystal Growth and Characterization of II-VI Compounds", University of Lancaster, U.K. April 14-16, 1980.

(4) 'Lattice Defects in $Hg_{1-x}Cd_xTe$ Alloys' I-Defect Structure of undoped and copper doped $Hg_{0.8}Cd_{0.2}Te$, H.R. Vydyanath and D.A. Nelson; submitted for publication in the Journal of Electrochemical Society.

(5) 'Lattice Defects in $Hg_{1-x}Cd_xTe$ Alloys' II-Defect Structure of Indium Doped $Hg_{0.8}Cd_{0.2}Te$, H.R. Vydyanath; submitted for publication in the Journal of Electrochemical Society.

(6) 'Lattice Defects in $Hg_{1-x}Cd_xTe$ Alloys' III-Defect Structure of Undoped $Hg_{0.6}Cd_{0.4}Te$, H.R. Vydyanath, J.C. Donovan and D.A. Nelson; submitted for publication in the Journal of Electrochemical Society.

(7) 'Doping behavior of Iodine in $Hg_{0.8}Cd_{0.2}Te$' H.R. Vydyanath; submitted for publication in the Journal of Electronic Materials.

III. TECHNICAL DETAILS

The work performed from July 1, 1980 to December 31, 1980 resulted in the establishment of a defect model for iodine doped $Hg_{0.8}Cd_{0.2}Te$. The technical details of the work are described in the form of a paper entitled 'Doping Behavior of Iodine Doped $Hg_{0.8}Cd_{0.2}Te$' which is being submitted to the Journal of Electronic Materials for publication. The paper describes the background material, the experimental details and analysis of the data. The mass action constant arrived at for the incorporation of iodine in $Hg_{0.8}Cd_{0.2}Te$ together with the values of the constants for the intrinsic excitation process and the incorporation of the doubly ionized native acceptor defect (established in one previous semiannual report) satisfactorily explains the experimental results for iodine doped $Hg_{0.8}Cd_{0.2}Te$ crystals.

III.1

DEFECT CHEMISTRY AND CHARACTERIZATION OF IODINE DOPED $Hg_{0.8}Cd_{0.2}Te$.

INTRODUCTION

With the emergence of $Hg_{1-x}Cd_xTe$ as a technologically useful infrared detector material,[1] it has become important to study in detail the nature of impurities and dopants in this material. As part of a program aimed at understanding the physicochemical properties of undoped and doped $Hg_{1-x}Cd_xTe$ compounds,[2] the defect structures of undoped $Hg_{0.8}Cd_{0.2}Te$, undoped $Hg_{0.6}Cd_{0.4}Te$, copper doped, and indium doped $Hg_{0.8}Cd_{0.2}Te$ were reported recently.[3-5] The present work was undertaken to extend such a defect structure investigation to iodine in $Hg_{0.8}Cd_{0.2}Te$. Halogens have been known to be donors occupying chalcogen lattice sites in II-VI compounds.[6] In the present work, the defect state prevailing in the iodine doped samples at the annealing temperatures is deduced from the Hall effect measurements on the crystals cooled to 77 K from the annealing temperatures. The results obtained are similar to those found for iodine doped CdS established from in situ high temperature Hall effect measurements previously;[7] iodine acts as a single donor occupying Te lattice sites, and as single acceptor paired with the native acceptor defects. The crystals are saturated with the metal iodide which influences the incorporation of the iodine donor species on tellurium sites as well as the iodine acceptor species, which result from the iodine on tellurium sites pairing with the doubly ionized native acceptor defects. The concentration of the iodine donor species increases with increase in the partial pressure of Hg, whereas that of the iodine acceptor species increases with decrease in the partial pressure of Hg. The equilibrium constants evaluated for the incorporation of the iodine donor and acceptor species as well as the iodine-Hg vacancy pairs satisfactorily explain the experimentally observed carrier concentration data.

EXPERIMENTAL

Iodine doped $Hg_{0.8}Cd_{0.2}Te$ crystal was grown by the solid state recrystallization method.[8] The total amount of iodine in the starting charge material was approximately 10^{20} cm^{-3}. Single crystal slices of $Hg_{0.8}Cd_{0.2}Te$ were cut from the larger boule. The slices were lapped down to thicknesses of less than 0.04 cm and were subsequently polished, etched in

Br methanol, and rinsed in DI water. The samples were annealed in evacuated quartz ampoules containing some Hg also to obtain the desired Hg pressure.[3] Typical anneal times used were 24 hours at temperatures of 600°C and higher, 3 days at 550°C, 7 days at 500°C, and 4 to 6 weeks at 450°C. These equilibration periods appeared satisfactory for the complete homogenization of the samples. Subsequent to the anneals at the high temperatures, the ampoules were quenched in ice water. Hall effect and electrical resistivity measurements were made using the van der Pauw technique.[9] Magnetic fields of 400 and 4000 gauss were used for the Hall effect measurements.

RESULTS

In order to ascertain an unambiguous evaluation of the carrier concentration, only those measurements where the Hall effect did not vary with the magnetic field were used in determining the carrier concentration in the samples.[3] The carrier concentration was calculated using the expression:

$$n \text{ or } p = \frac{1}{|R_H q|}$$

The hole concentration in the p-type samples and the electron concentration in the n-type samples did not vary with the temperature of measurement varying from 77 K to 145 K, thus indicating that the iodine donor species as well as the iodine acceptor species and the native acceptor defect species are all ionized at 77 K; all the carrier concentration measurements were carried out at 77 K to deduce the defect state at the annealing temperatures.

Figure 1 shows the carrier concentration at 77 K in the iodine doped samples as a function of the partial pressure of Hg at the various annealing temperatures. It is apparent from the figure that the samples are n-type under Hg rich conditions whereas they turn p-type at lower Hg pressures similar to the observation in the indium doped samples.[4] Also, the electron concentration appears to increase with increase in the Hg pressure just as was observed for the indium doped samples.[4]

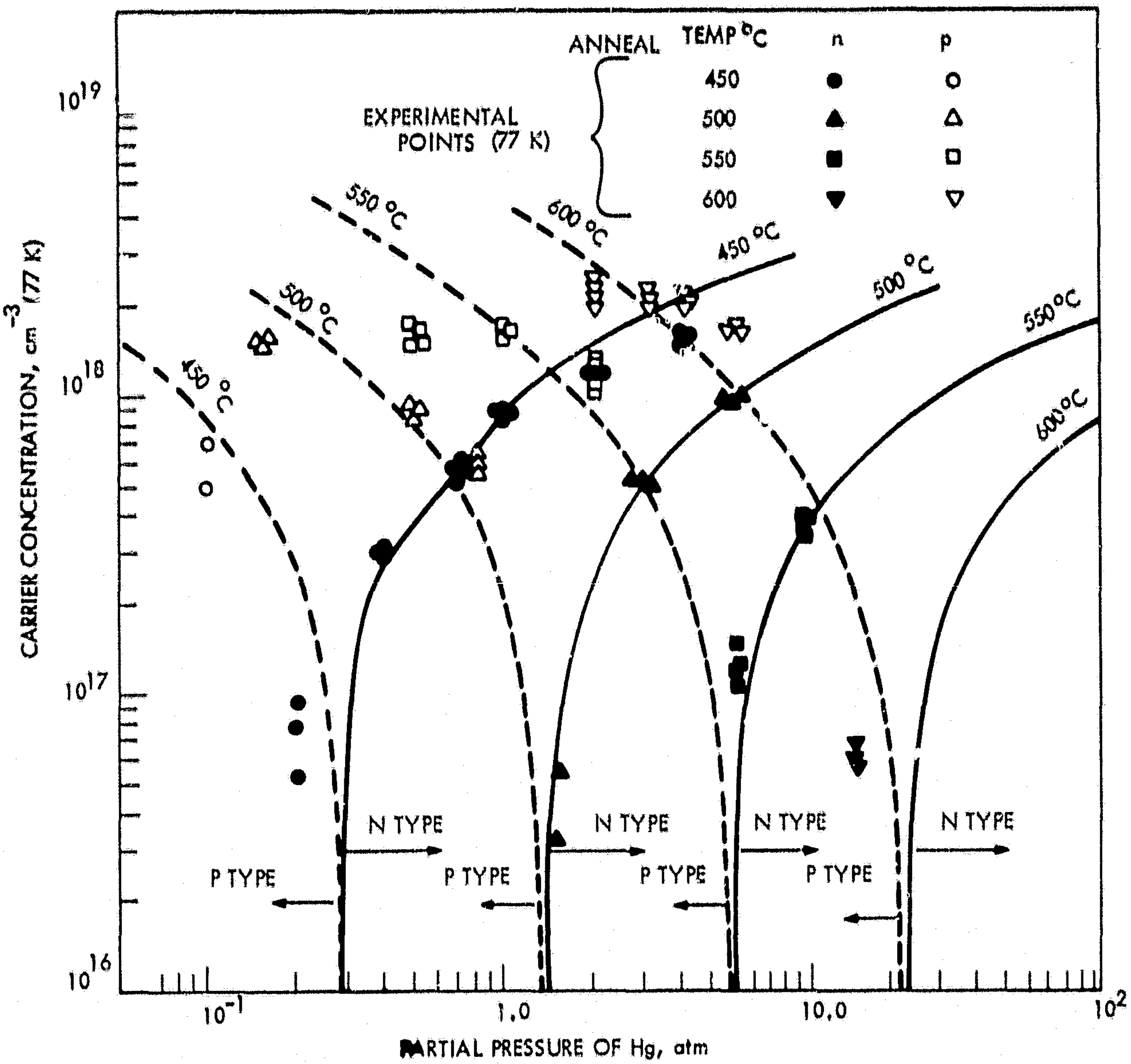

Figure 1. Carrier Concentration at 77K as a Function of the Partial Pressure of Hg for Iodine doped $Hg_{0.8}Cd_{0.2}Te$ Samples Annealed at Various Temperatures and Quenched to Room Temperature; Solid Lines Show the Calculated Electron Concentrations While the Dashed Lines show the Calculated Hole Connections.

Figure 2 shows the electron mobility at 77 K as a function of the electron concentration in the samples. The magnitude of the electron mobility is similar to that observed in the indium doped samples[4] for comparable electron concentrations.

DISCUSSION

Iodine can exist in three forms, namely as a single donor occupying Te lattice sites $I_{Te}^{\bullet}$ or as single acceptor present either interstitally I_i' or paired with the doubly ionized native acceptor defects as $(I_{Te}V_{Hg})'$. The following interferences can be drawn from the experimental data:

1. The concentration of iodine in the starting charge was on the order of 10^{20} cm^{-3}, whereas the maximum electron concentration in the doped samples is only on the order of 10^{18} cm^{-3}.

2. The concentration of electrons obtained at 77 K is less than the intrinsic carrier concentration[3] at the annealing temperatures.

3. The concentration of electrons increases with increase in the Hg pressures.

4. The hole concentration in the p-type samples at low Hg pressures is close to that obtained in the undoped samples.[3]

Several defect situations can be considered to explain the experimental data:

1. $[I_{Te}^{\bullet}] = [I_{TOT}]$ = constant and the crystal is intrinsic at the annealing temperatures. In the cooled crystals $[e'] = [I_{Te}^{\bullet}] >> [V_{Hg}'']$. Such a model would predict an electron concentration independent of the partial pressure of Hg particularly at lower temperatures and higher Hg pressures for which conditions the native acceptor defect concentra-

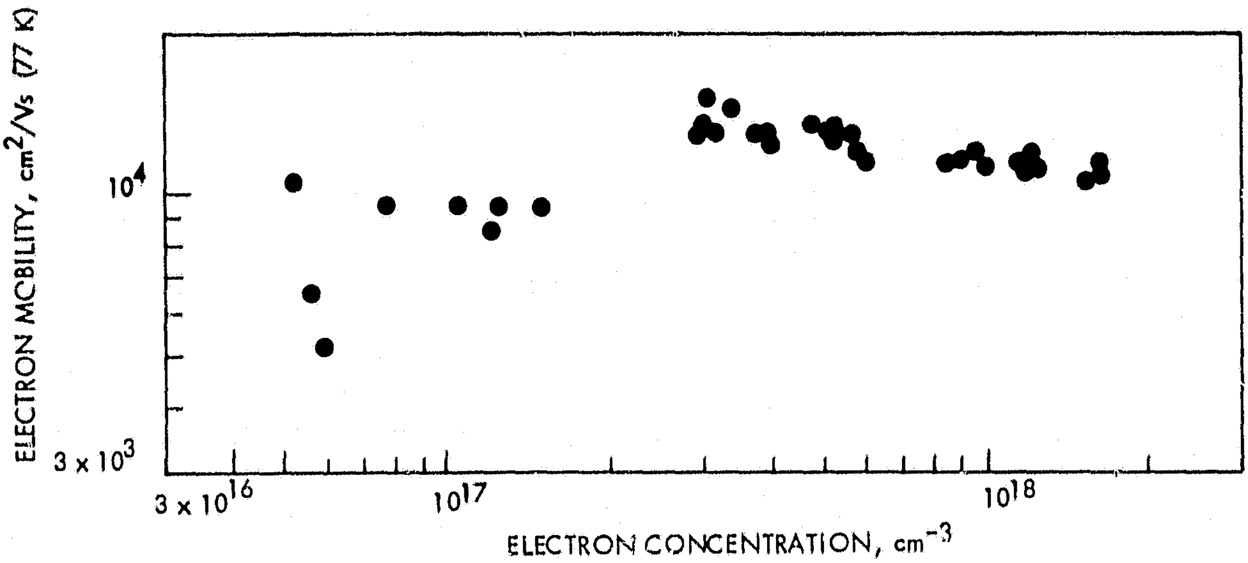

Figure 2. Electron Mobility at 77K as a Function of the Electron concentration for the Iodine Doped $Hg_{0.8}Cd_{0.2}Te$ Samples.

tion is expected to be less than the concentration of the electrons obtained in the crystals. The experimental data are in disagreement with this model.

2. $[I_{Te}^{\bullet}]$ = $[(I_{Te}V_{Hg})']$ $\approx$ $[I_{TOT}/2]$ and the crystal is intrinsic at the annealing temperatures. In the crystals cooled to 77 K, $[e']$ = $[I_{Te}^{\bullet}]$ minus $[I_{Te}V_{Hg})']$. This model predicts an independence of the electron concentration as a function of the partial pressure of Hg particularly at the highest Hg pressures contrary to the observed results.

3. The crystals are saturated with iodine with the formation of $(Hg,Cd)I_2$ as the second phase. The concentration of $I_{Te}^{\bullet}$ as well as $(I_{Te}V_{Hg})'$ depends on the partial pressure of Hg with $[I_{Te}^{\bullet}]$ varying as $pHg^{+1/2}$ and $[(I_{Te}V_{Hg})']$ varying as $pHg^{-1/2}$. The incorporation reactions of interest are:

A. $Hg(g) + (Hg,Cd)I_2(s) \rightarrow 2\, I_{Te}^{\bullet} + 2e' + 2Hg_{Hg}^{x}$

$$K_{I_{Te}} = [I_{Te}^{\bullet}]^2\ [e']^2/p_{Hg}\, a_{(Hg,Cd)I_2} \qquad (1)$$

where $a(Hg,Cd)I_2$ refers to the activity of the $(Hg,Cd)I_2(s)$ phase.

For an intrinsic crystal $[e']$ = $[h^{\bullet}]$ = $\sqrt{K_i}$. Since the crystal is saturated with iodine and $(Hg,Cd)I_2$ exists as a pure second phase, $a(Hg,Cd)I_2$, the activity of the metal iodide is unity and hence $[I_{Te}^{\bullet}]$ α $pHg^{1/2}$ from mass action relation (1).

B. $2e' + (Hg,Cd)I_2(s) \rightarrow 2(I_{Te}V_{Hg})' + Hg(g)$

$$K_{I_{Te}V_{Hg}} = [(I_{Te}V_{Hg})']^2\ pHg/[e']^2\ a(Hg,Cd)I_2 \qquad (2)$$

For an intrinsic crystal with

$[e'] = [h^\bullet] = \sqrt{K_i}$ and $a_{(Hg,Cd)I_2} = 1$ for a pure second phase of $(Hg,Cd)I_2$

$[(I_{Te}V_{Hg})'] \propto p_{Hg}^{-1/2}$ from mass action relation (2).

This last model is similar to that established for iodine doped CdS[7] where CdI_2 was assumed to be present as a pure second phase. Similarity between the indium doping[4] and iodine doping in $Hg_{0.8}Cd_{0.2}Te$ is also worth noting. In the indium doped crystals the samples are intrinsic at the annealing temperature with the electron concentration increasing with increasing Hg pressure; however, $In_2Te_3(s)$ that is in equilibrium with $Hg_{0.8}Cd_{0.2}Te(s)$ is present as a solid solution of In_2Te_3 in $Hg_{0.8}Cd_{0.2}Te$ and hence $a_{In_2Te_3}$ the activity of the metal telluride is variable depending on the amount of the total indium present in the crystals whereas in the present case $(Hg,Cd)I_2$ is assumed to be present as a pure second phase and hence $a_{(Hg,Cd)I_2}$, the activity of the metal iodide is taken to be unity.

It should be also mentioned that iodine in interstitial sites can be considered for the acceptor species instead of $(I_{Te}V_{Hg})'$ pairs. The incorporation reaction can then be written as:

$$\text{C.}\quad 2e' + (Hg,Cd)I_2(s) \rightarrow 2I_i' + Hg(g)$$

$$K_{I_i} = [I_i']^2\, p_{Hg}/[e']^2\, a_{(Hg,Cd)I_2} \qquad (3)$$

For $[e'] = [h^\bullet] = \sqrt{K_i}$ and $a_{(Hg,Cd)I_2} = 1$ for a pure second phase of $(Hg,Cd)I_2$

$[I_i'] \propto p_{Hg}^{-1/2}$ from mass action relation (3) similar to the variation of $[I_{Te}V_{Hg})']$ as a function of p_{Hg} deduced from mass action (2) earlier. Owing to the large ionic radius of the iodine atoms, its presence in interstitial sites in large concentrations is questionable and hence, in further discussions $(I_{Te}V_{Hg})'$ will be considered to be the dominant iodine acceptor species rather than I_i'.

ANALYSIS OF THE CARRIER CONCENTRATION IN THE COOLED CRYSTALS

The various species to be considered in the electroneutrality condition are e', $h^{\cdot}$, V''_{Hg}, $I^{\bullet}_{Te}$ and $(I_{Te}V_{Hg})'$. Apart from the defect reactions A and B written earlier for the incorporation of $I^{\bullet}_{Te}$ and $(I_{Te}V_{Hg})'$ the other defect reactions to be considered are:

D. $0 \rightarrow e' + h^{\cdot}$

$$K_i = [e'] [h^{\cdot}] \qquad (4)$$

E. $Hg^{X}_{Hg} \rightarrow V''_{Hg} + 2h^{\cdot} + Hg(g)$

$$K''_{VHg} = [V''_{Hg}] [h^{\cdot}]^2 \, p_{Hg} \qquad (5)$$

The complete electroneutrality condition is written as:

$$[e'] + 2 [V''_{Hg}] + [(I_{Te}V_{Hg})'] = [I^{\cdot}_{Te}] + [h^{\cdot}] \qquad (6)$$

Expressing the various species in terms of the mass action constants defined in relations 1 through 5 we get:

$$[e'] + 2K''_{VHg} \, p^{-1}_{Hg} \, [e']^2 \Big/ K_i^{\,2} + K^{1/2}_{I_{Te}V_{Hg}} \, [e'] \, p^{-1/2}_{Hg}$$

$$- K^{1/2}_{I_{Te}} \, p^{1/2}_{Hg} \Big/ e' - K_i \Big/ e' = 0 \qquad (7)$$

with some simplification we get:

$$[e']^3\, 2K''_{VHg} p^{-1}_{Hg}/K_i^{\,2} + [e']^2 \left(1 + K^{1/2}_{I_{Te}V_{Hg}} p^{-1/2}_{Hg}\right) = K^{1/2}_{I_{Te}} p^{1/2}_{Hg} + K_i \qquad (8)$$

In the crystals cooled to 77 K

$$[e']_{77\ K} \text{ or } [h^\bullet]_{77\ K} = \left| [I^\bullet_{Te}] - 2[V''_{Hg}] - [(I_{Te}V_{Hg})'] \right| \qquad (9)$$

The concentrations $[V''_{Hg}]$, $[(I_{Te}V_{Hg})']$ and $[I^\bullet_{Te}]$ in Equation (9) are given by the second, third, and fourth terms of Equation (7), respectively. Of the four mass action constants in Equations (7) and (8), values of the two constants K_i and K''_{VHg} are known from the work on the undoped crystals[3] and are given by

$$K_i = 9.16 \times 10^{40} \exp(-0.57\ \mathrm{eV}/kT)\ \mathrm{cm}^{-6} \qquad (10)$$

$$K''_{VHg} = 1.58 \times 10^{69} \exp(-2.24\ \mathrm{eV}/kT)\ \mathrm{cm}^{-9}\ \mathrm{atm} \qquad (11)$$

The values of the constants $K_{I_{Te}}$ and $K_{I_{Te}V_{Hg}}$ were optimized by a procedure of trial and error until the calculated carrier concentration as given by Equation (9) agreed best with the experimental results, as a function of the partial pressure of Hg at various temperatures. The values of the mass action constants $K_{I_{Te}}$ and $K_{I_{Te}V_{Hg}}$ established from the present work are given by

$$K_{I_{Te}} = 5.29 \times 10^{31} \exp(0.717\ \mathrm{eV}/kT)\ \mathrm{cm}^{-12}\ \mathrm{atm}^{-1} \qquad (12)$$

and

$$K_{I_{Te}V_{Hg}} = 2.67 \times 10^{35} \exp(-0.593\ \mathrm{eV}/kT)\ \text{atmosphere} \qquad (13)$$

The calculated defect concentrations as a function of the partial pres[illegible]f Hg at various temperatures are shown in Figure 3 through 6; the experimentally obtained carrier concentrations are also shown in the figures. The agreement between the calculated values and the experimental results appears satisfactory except near the p-n transition points. Inadequate quenching can explain the discrepancy somewhat. Near p-n transition $[I_{Te}^{\bullet}] = 2\ [V_{Hg}'']+[(I_{Te}V_{Hg})']$. If the quenching is inadequate, the sample may spend sufficient time at a lower temperature (between room temperature and the anneal temperature) where the pairing reaction between $I_{Te}^{\bullet}$ and V_{Hg}'' is promoted with the result that the partial pressure of Hg at which p-n transition occurs moves to lower Hg pressures. As can also be noted from the figures, the concentration of the iodine donor species increases with increase in the partial pressure of Hg whereas the vice versa is true for the iodine acceptor species. The concentration of the native acceptor defects is essentially the same as in the undoped crystals[3] since the concentration of iodine in the crystals is insufficient to make them extrinsic; the crystals are intrinsic just as the undoped crystals are under similar physicochemical conditions.[3]

PAIRING BETWEEN $I_{Te}^{\bullet}$ and V_{Hg}''

The pairing reaction between the singly positively charged iodine donor species and the doubly negatively charged native acceptor defect species is written as:

$$\text{F.}\quad I_{Te}^{\bullet} + V_{Hg}'' \rightarrow (I_{Te}V_{Hg})'$$

$$K_{p(I_{Te}V_{Hg})} = [(I_{Te}V_{Hg})'] \,/\, [I_{Te}^{\bullet}]\ [V_{Hg}'']$$

If we believe the iodine acceptor species to be $(I_{Te}V_{Hg})'$, then from mass action relations 1 through 5, we get

$$K_{p(I_{Te}V_{Hg})} = \left(\frac{K_{I_{Te}V_{Hg}}}{K_{I_{Te}}}\right)^{1/2} \frac{K_i^{\,2}}{K''_{VHg}}$$

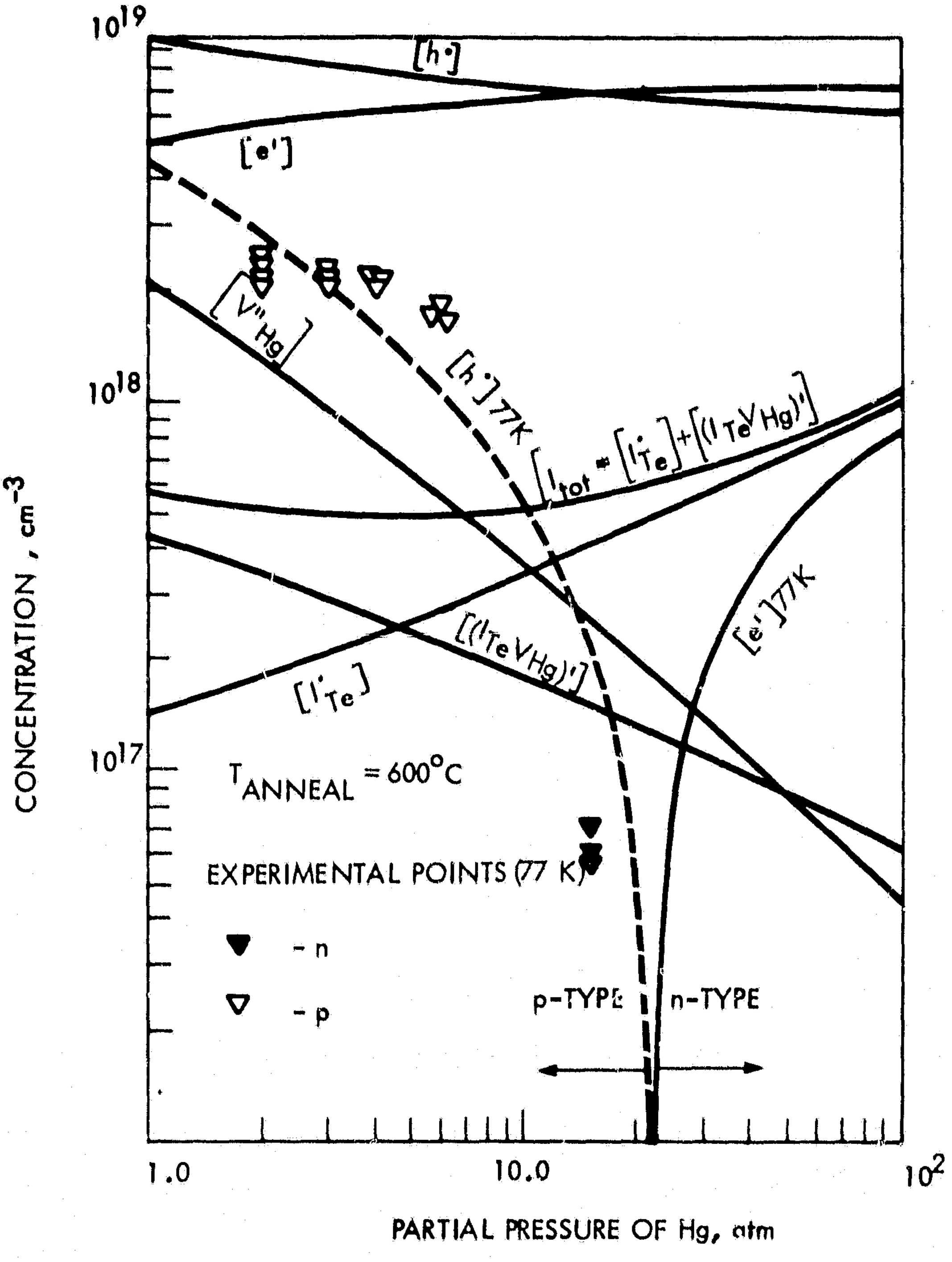

Figure 3. Calculated defect concentrations ($[e']$, $[h^{\bullet}]$, $[I^{\bullet}_{Te}]$, $[(I_{Te}V_{Hg})']$ and $[V''_{Hg}]$) as a function of the partial pressure of Hg for iodine doped $Hg_{0.8}Cd_{0.2}Te$ annealed at 600°C and quenched to room temperature; calculated electron and hole concentrations expected at 77 K (indicated by solid and dashed lines respectively) are also shown along with the experimental points.

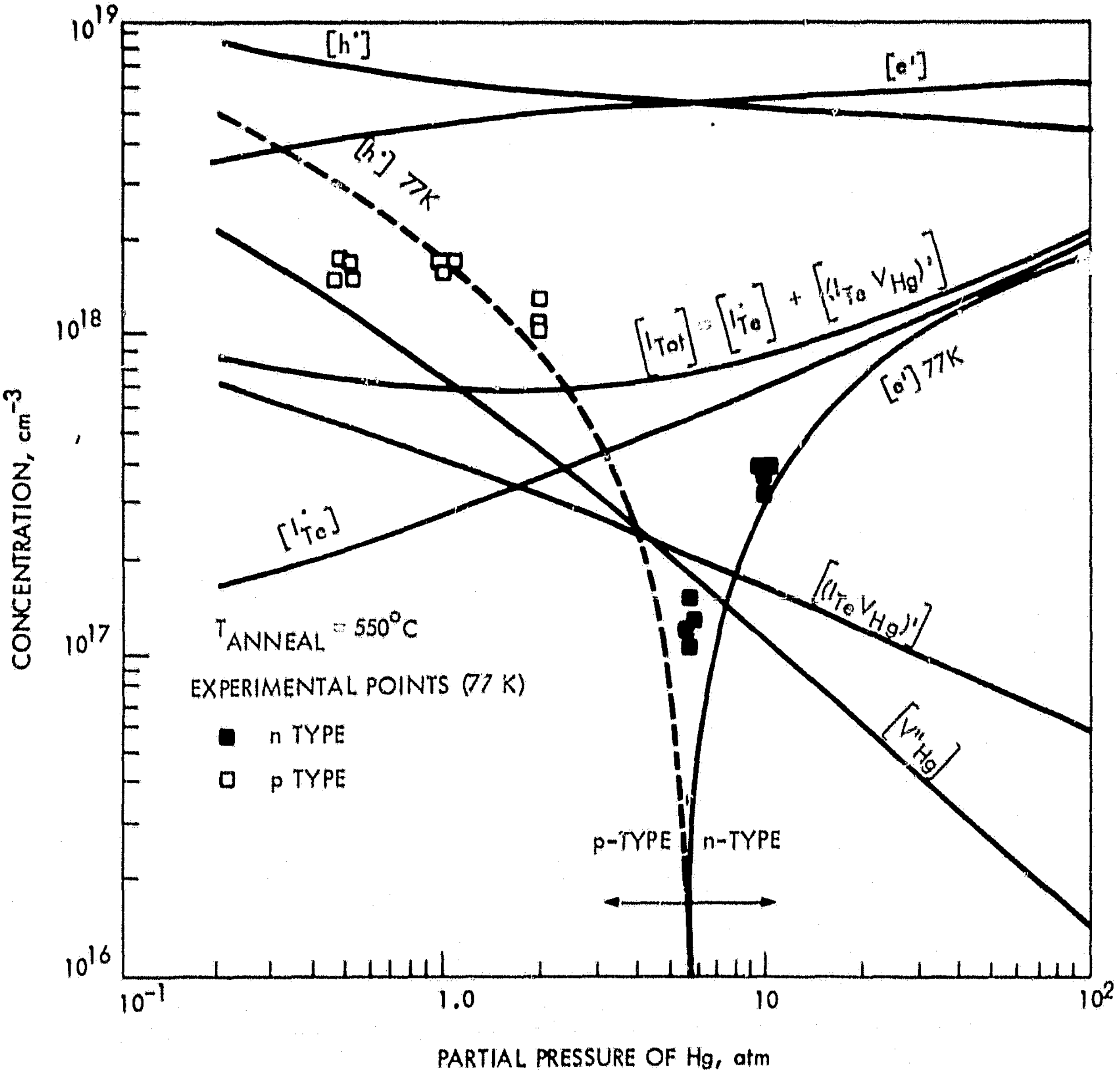

Figure 4. Calculated defect concentrations ($[e']$, $[h^{\cdot}]$, $[I^{\bullet}_{Te}]$, $[(I_{Te}V_{Hg})']$ and $[V''_{Hg}]$) as a function of the partial pressure of Hg for iodine doped $Hg_{0.8}Cd_{0.2}Te$ annealed at 550°C and quenched to room temperature; calculated electron and hole concentrations expected at 77 K (indicated by solid and dashed lines respectively) are also shown along with the experimental points.

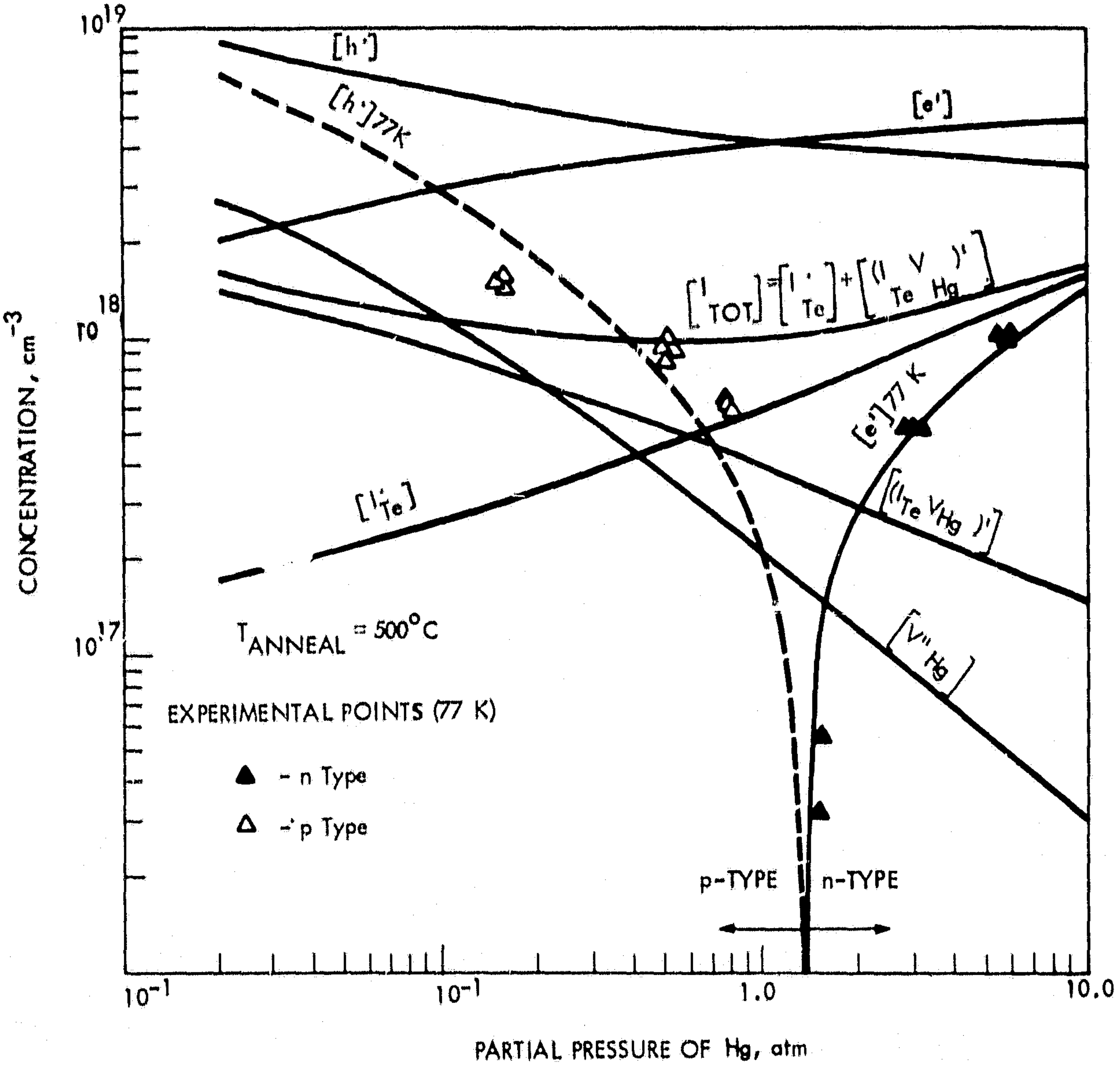

Figure 5. Calculated defect concentrations ($[e']$, $[h^{\bullet}]$, $[I^{\bullet}_{Te}]$, $[(I_{Te}V_{Hg})']$ and $[V''_{Hg}]$) as a function of the partial pressure of Hg for iodine doped $Hg_{0.8}Cd_{0.2}Te$ annealed at 500°C and quenched to room temperature; calculated electron and hole concentrations expected at 77 K (indicated by solid and dashed lines respectively) are also shown along with the experimental points.

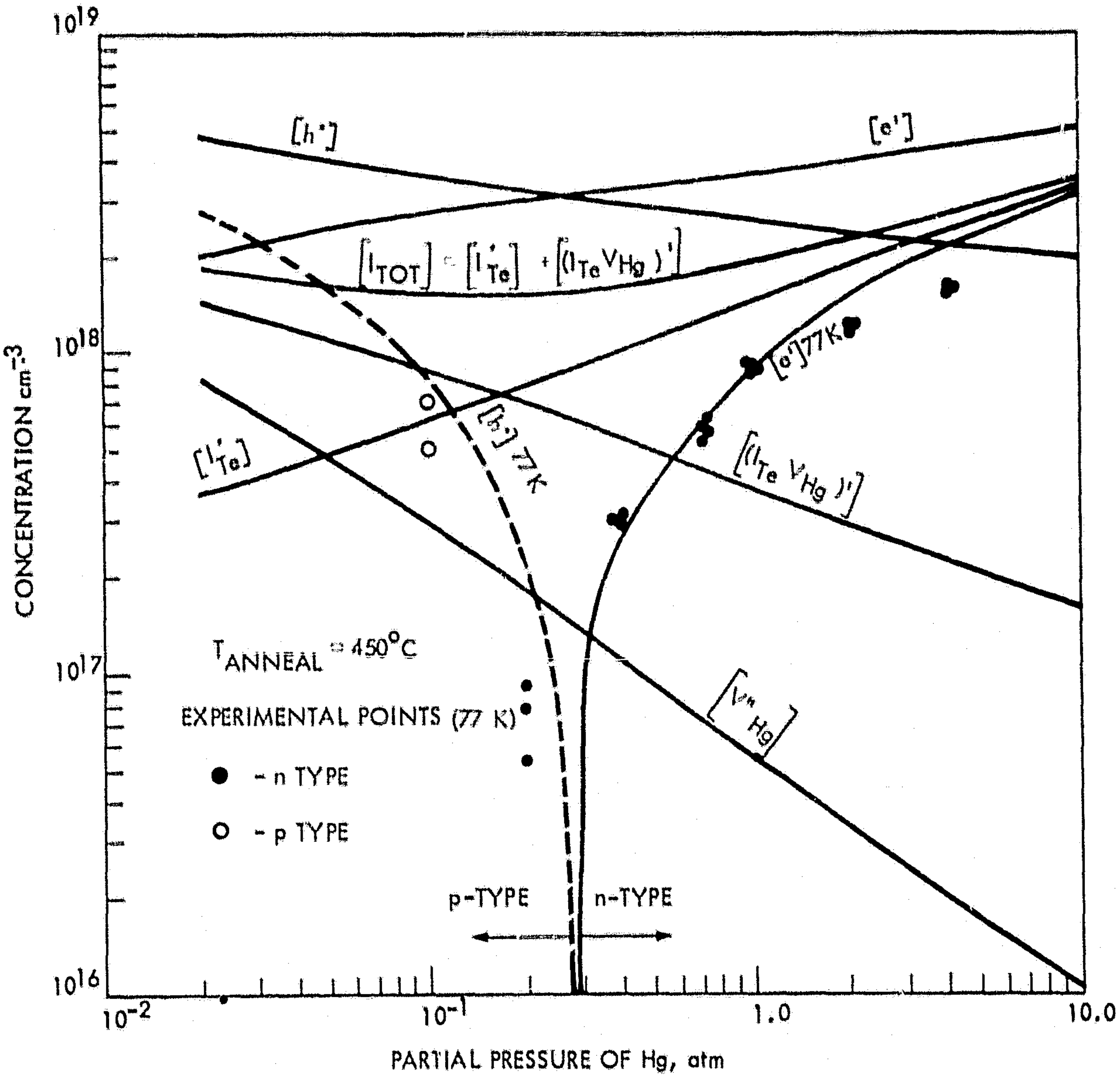

Figure 6. Calculated defect concentrations ([e'], [h·], [$I^{\bullet}_{Te}$], [$(I_{Te}V_{Hg})'$] and [V''_{Hg}]) as a function of the partial pressure of Hg for iodine doped $Hg_{0.8}Cd_{0.2}Te$ annealed at 500°C and quenched to room temperature; calculated electron and hole concentrations expected at 77 K (indicated by solid and dashed lines respectively) are also shown along with the experimental points.

With the values of K_i, $K_{V''_{Hg}}$, and $K_{I_{Te}V_{Hg}}$ from expressions (10) through (13) we evaluate

$$K_p(I_{Te}V_{Hg}) = 2.77 \times 10^{-21} \exp (0.445 \text{ eV/kT}) \text{ cm}^3 \tag{15}$$

$$= 55.8 \exp (0.445 \text{ eV/kT}) (\text{Site Fr})^{-1} \tag{16}$$

COULOMBIC VALUE FOR THE PAIRING ENTHALPY

The pairing constant is written as:

$$K_p = K_p^{\circ} \exp (-H_p \text{ eV/kT}) (\text{Site Fr})^{-1}$$

Hp, the enthalpy of pairing can be calculated on the basis of coulombic attraction between $I_{Te}^{\bullet}$ and V''_{Hg}

$$H_p = \frac{-2q^2}{\varepsilon r} \qquad [10]$$

where ε is the static dielectric constant, r is the distance between $I_{Te}^{\bullet}$ and V''_{Hg}. The factor 2 arises because of the double charge on V''_{Hg}. For $Hg_{0.8}Cd_{.2}Te$, $\varepsilon \approx 17.5$ [1] and $r_{Hg\text{-}Te} = 2.8A^{\circ}$ ($\sqrt{3/4}$ times $a_0 = 6.46A^{\circ}$). The calculated value based on the coulombic calculations turns out to be

$$H_p = -0.581 \text{ eV}$$

This value is deemed to be close to the value of -0.445 eV [expressions (15) and (16)] calculated by us from the experimental data.

SOLID SOLUBILITY OF IODINE IN $Hg_{0.8}Cd_{0.2}Te$

The carrier concentration data shown in Figure 1 indicate an increase of electron concentration at 77K with decrease in the annealing temperature for comparable Hg pressures, implying an increase of the solubility of the iodine donor species with decrease in temperature. Fearing that complete equilibration may not have been attained at the lower temperatures, (particularly with regard to the iodine species) Hall effect measurements were carried out on several samples which were thermally cycled from the lower temperature to higher temperatures and vice versa; the resulting carrier concentrations were independent of the prior thermal history thus confirming the validity of the experimental results of Figure 1 showing a negative temperature dependence of the solubility of iodine in $Hg_{0.8}Cd_{0.2}Te$. The calculated defect isotherms shown in Figures 3 through 6 do predict an increase of the total amount of iodine in solid solution of $Hg_{0.8}Cd_{0.2}Te$ ($[I_{Tot}] = [I^{\bullet}_{Te}] + [(I_{Te}V_{Hg})']$) with decrease in temperature thus accounting for the experimental results of Figure 1.

ELECTRON MOBILITY

The values of electron mobility shown in Figure 2 for the iodine doped samples are comparable to those obtained for indium doped samples[4] for similar electron concentrations. The data in Figure 2 appear to indicate that the mobility initially increases with decrease in electron concentration, and decreases with decrease in electron concentration for electron concentrations less than about 2×10^{17} cm^{-3}. A qualitative explanation for this can be elucidated from the defect concentration isotherms shown in Figures 3 through 6. As can be noted from these figures, for electron concentrations greater than 2×10^{17} cm^{-3} the doubly ionized native acceptor defect concentration is negligible compared to the singly ionized Iodine species and the mobility is essentially dominated by the iodine species, and thus the mobility decreases with increasing electron concentrations originating from increasing iodine donor concentration. For electron concentrations less than 2×10^{17} cm^{-3}, the concentration of the doubly ionized native acceptor defects (V''_{Hg}) becomes dominant enough to contribute to ionized impurity scattering. Since these centers are four times as strong scatterers as the singly ionized iodine species, the electron mobility decreases with increase in the concentration of these native acceptor defects and thereby with decrease in electron concentration.

CONCLUSION

Iodine acts as a single donor occupying tellurium lattice sites ($I_{Te}^{\bullet}$) and as an acceptor $(I_{Te}V_{Hg})'$ paired with the doubly ionized native acceptor defects. Equilibrium constants have been evaluated for the incorporation of the iodine species as well as for the iodine-native acceptor defect pairing.

ACKNOWLEDGEMENT

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IV. SUMMARY

The work performed on this program so far has resulted in the establishment of the defect modules for undoped $Hg_{0.8}Cd_{0.2}Te$ and undoped $Hg_{0.6}Cd_{0.4}Te$. The mechanism of incorporation of copper, indium and iodine in $Hg_{0.8}Cd_{0.2}Te$ have also been established. In the next semiannual report, the details of incorporation of phosphorous in $Hg_{0.8}Cd_{0.2}Te$ will be discussed.

REFERENCES

1. R. Dornahaus and G. Nimtz, Solid State Physics, Vol. 78, Springer-Verlag, New York (1976).

2. H.R. Vydyanath, "Defect Chemistry and Characterization of (Hg,CD)Te" Semiannual technical report to NASA, George C. Marshall Space Flight Center, Alabama, under contract NAS8-33245, June 1980 (unpublished).

3. H.R. Vydyanath and D.A. Nelson (Submitted for publication in the Journal of Electrochemical Society).

4. H.R. Vydyanath, (Submitted for publication in the Journal of Electrochemical Society).

5. H.R. Vydyanath, J.C. Donovan, and D.A. Nelson (Submitted for publication in the Journal of Electrochemical Society).

6. K. Zanio, "Semiconductors and Semimetals" Vol. 13 (Willardson and Beer Eds), Academic Press, New York, (1978) p. 129.

7. H.R. Vydyanath, S.S. Chern, and F.A. Kröger, J. Phys, Chem. Solids 3[illegible], 1317 (1973).

8. D.A. Nelson, W.M. Higgins, and R.A. Lancaster, Proc. SPIE, 225, 48 (1980).

9. L.J. Van Der Pauw, Philips Tech. Rev. 20, 220 (1959).

10. F.A. Kröger "The Chemistry of Imperfect Cyrstals" Second revised edition, Volume 2, Chapter 10. North Holland (1974).