

Vapor Pressure Scanning of Nonstoichiometry in CdTe

J. H. GREENBERG,* V. N. GUSKOV, V. B. LAZAREV,
AND O. V. SHEBERSHNEVA

*Kurnakov Institute of General and Inorganic Chemistry, Academy of
Sciences, 117907 Moscow, Leninski prosp. 31, Russia*

Received February 19, 1992; in revised form June 22, 1992; accepted June 29, 1992

Results of vapor pressure scanning of the cadmium telluride solidus surface are reported. The deviation from stoichiometry is found to be up to $(0.6-13.8) \times 10^{-3}$ at.% at temperatures from 945 to 1360 K and vapor pressures from 2.3 to 87.2 kPa on the tellurium side, while that on the cadmium side is $(0.1-3.3) \times 10^{-3}$ at.% in the temperature and vapor pressure ranges from 695 to 992 K and from 0.5 to 57.3 kPa, respectively. The position of the congruent sublimation curve in the P - T - X phase space is discussed and some specifics of the solidus surface are outlined. The maximum congruent sublimation temperature was found to be 1324 K, 41 K lower than the maximum melting point of CdTe. $P(\text{Cd})$ - T and $P(\text{Te}_2)$ - T projections of the Cd-Te phase diagram are presented. Partial molar enthalpies and entropies of the component elements are deduced for cadmium telluride. © 1993 Academic Press, Inc.

Introduction

CdTe is one of the more important semiconductors. The properties of this material are strongly dependent on the actual composition of the crystal. Hence to realize fully the potentials of the material it is crucial to know the maximum nonstoichiometry of this compound and to design appropriate technological ways of achieving the desired stoichiometry. According to recent reviews (1, 2), both components display retrograde solubility in CdTe with maxima of 10^{-3} at.% at 1353 K for Te nonstoichiometry and at 1253 K for Cd-saturated CdTe. These values were obtained either from indirect experiments under ambient conditions (e.g., Hall effect measurements on quenched samples of various compositions) or from calcula-

tions based on a quasi-chemical theory of defects (1, 3). No direct experimental data on high-temperature nonstoichiometry in CdTe have yet been published.

We report experimental results of vapor pressure scanning of the CdTe solidus surface which sets the boundary for the single-phase volume of this crystalline compound in the P - T - X phase space.

Experimental

The experimental equipment for vapor pressure measurements in a closed volume was described in detail in our earlier publications, e.g., (4). It was calibrated against the standard saturated vapor pressures of liquid Cd metal. The experimental Third Law standard enthalpy of vaporization was found to be 112.3 ± 1.0 kJ/mole, in good agreement with the tabulated value of $112.05 \pm$

* To whom correspondence should be addressed.

0.63 kJ/mole (5). In addition, the unsaturated vapor pressure of Cd was also measured, and the evaporated mass was calculated from these data. It corresponded to the weighed mass to within 1×10^{-4} g. Pressures up to 100 kPa were read with a precision of 10 Pa. The initial alloys were prepared by heating the high-purity elements loaded into the quartz carbon-coated reaction vessel of a measured volume. In several experiments the samples were placed in a carbon crucible. The typical total mass of the sample was about 50 g, weighed with a precision of 5×10^{-5} g. The reaction bulb with the charge was evacuated ($\approx 10^{-3}$ Pa) and sealed. It was heated in a vertical furnace under vibration, with 12-hr isothermal periods at the melting temperatures of both elements. The bulb was then slowly heated to the melting point of CdTe (or 100 K lower), held there for 24 hr, cooled to 730 K at the rate of 20 K/hr, held at this temperature for 48 hr, and finally cooled to room temperature (20 K/hr). This bulb served as a reaction vessel for the Bourdon gauge in the vapor pressure measurements. A total of 26 samples with initial compositions from 49.94 to 50.04 at.% Te were investigated.

Special care was taken to ensure that equilibrium was reached at every experimental point. For this purpose time dependencies of the vapor pressure were examined at constant temperatures. The time limit was from 0.5 to 60 hr. It was shown that vapor pressure remained unchanged after 0.5 to 1 hr exposure at a constant temperature. In addition, cooling and heating curves were compared, and no significant differences were observed.

Results

Nonstoichiometry

To determine the composition of the crystal in equilibrium with the vapors, the total vapor pressure was measured in a closed

bulb of a known volume at different temperatures. It was shown (1-3) that for CdTe there was a minimum total vapor pressure in the two-phase solid-vapor equilibrium, which corresponded to the congruent sublimation $S(\text{CdTe}) = V$. This congruent sublimation curve divides the sublimation region into two parts: VS, where the vapor V is enriched in Cd compared to the Cd-saturated solid S; and SV, where the crystal is Te-saturated (the sequence of phases in phase equilibria adopted in this paper will follow the Te content in the phases).

The composition of the crystal X_S in equilibrium with the vapor can be determined at every experimental (P, T) point by subtracting the number of gram-atoms $n(i)$ of the elements, evaporated at this temperature, from the number of gram-atoms $N(i)$ in the initial sample:

$$X_S \text{ (at.\% Te)} = \frac{N(\text{Te}) - n(\text{Te})}{[N(\text{Te}) + N(\text{Cd})] - [n(\text{Te}) + n(\text{Cd})]} \cdot 100\%. \quad (1)$$

To do this one should know the partial pressures of all the vapor species. No heteroatomic gaseous molecules were observed in the mass spectra of CdTe (6); the only Cd species is Cd(g), whereas tellurium forms seven gaseous polymers Te_k , $k = 1$ to 7 (7). Hence

$$n(\text{Cd}) = P(\text{Cd})V/RT \quad (2)$$

$$n(\text{Te}) = (V/RT) \sum_{k=1}^7 kP(\text{Te}_k) \quad (3)$$

and the total vapor pressure P , measured at every temperature T , is a sum of eight partial pressures:

$$P = P(\text{Cd}) + \sum_{k=1}^7 P(\text{Te}_k). \quad (4)$$

To calculate these partial pressures, eight independent equations are necessary. One

of them is Eq. (4); six more are provided by the equilibrium constants of the polymerization reactions

$$\begin{aligned} \text{Te}_k &= k/2 \text{Te}_2 \\ &\vdots \\ K_j &= P^{k/2}(\text{Te}_2)/P(\text{Te}_k). \end{aligned} \quad (5-10)$$

The K_j values can be calculated by a standard procedure from $R \ln K_j = \Delta\Phi_j^\circ - \Delta H_{\text{O}_f}^\circ/T$ at any temperature since the $\Delta\Phi_j^\circ$ and $\Delta H_{\text{O}_f}^\circ$ values are tabulated for all the Te_k polymers (7). The eighth equation is the relation between $P(\text{Cd})$ and $P(\text{Te}_2)$ determined by the Gibbs free energy of formation of CdTe ,

$$\Delta G_T^\circ = RT \ln [a(\text{Cd})a^\alpha(\text{Te})], \quad (11)$$

where $\alpha = X_S/(1 - X_S)$. It was assumed that at $T = \text{const}$ ΔG_T° remains constant within the homogeneity range of CdTe which deviates only slightly from $X_S = 0.5$. The partial pressures are readily calculated from the activities $a(i)$ since the saturated vapor pressures for pure $\text{Cd}(1)$ and $\text{Te}(1)$ are known (5, 7). Thus the vapor pressure problem of determining the composition of the crystalline cadmium telluride in the solid-vapor equilibrium at a fixed temperature consists of solving a set of eight equations (4-11) with eight unknown partial pressures and calculating X_S from Eq. (1). The composition of the equilibrium vapor X_V is then calculated from

$$X_V (\text{at.}\% \text{ Te}) = \frac{n(\text{Te})}{n(\text{Te}) + n(\text{Cd})} \cdot 100\%. \quad (12)$$

In these calculations the values of $\Phi_j^\circ(\text{Cd},g)$ and $\Phi_j^\circ(\text{CdTe},s)$ were taken from the IV-TANTERMO data base (7).

As a result of this treatment each experimental (P,T) point produces in the solid-vapor equilibrium a pair of scanning points, (P,T,X_S) and (P,T,X_V) , on the solidus S and vaporus V surfaces. Correspondingly, the

entire experimental data file $\{P,T\}$, treated in this way, results in two sets of scanning points, $\{P,T,X_S\}$ and $\{P,T,X_V\}$, with one-to-one correspondence, which outline the position of the solidus and vaporus conjugated surfaces in the $P-T-X$ phase space.

When the boundary of the homogeneity range of CdTe is reached during the vapor pressure experiment, a break in the (P,T) curve which corresponds to the change in the phase state of the system, e.g., two-phase to three-phase transition, is observed. To determine the $P-T-X$ coordinates of this point (which actually is the maximum nonstoichiometry), $P-T$ and $T-X$ projections of the experimental curves were obtained in an analytical form $P = f(T)$; $X_S = \psi(T)$. The temperature and vapor pressure at the boundary of the homogeneity range can be calculated from the set of equations

$$\begin{aligned} P &= f(T) \\ P &= \varphi(T), \end{aligned} \quad (13)$$

where $P = \varphi(T)$ is the temperature dependence of the vapor pressure on the three-phase equilibrium SLV, or VLS reported earlier (8) for the entire $P-T-X$ range of CdTe stability. The corresponding composition X_S can then be calculated from the individual $X_S = \psi(T)$ polynomials at temperatures calculated from Eqs. (13). The results are given in Table I and Fig. 1. The solid line in Fig. 1 is a best fit of the experimental data. It can be seen that the solidus is strongly asymmetrical, the maximum Cd nonstoichiometry being almost an order of magnitude less than that of Te, and the stoichiometric plane $X = 50 \text{ at.}\%$ is within the single-phase volume.

$P(\text{Te}_2)-T$ and $P(\text{Cd})-T$ projections of the cadmium telluride range of stability are given in Figs. 2 and 3. The partial pressures in three-phase equilibria were calculated from Eq. (11) and the measured total vapor pressures from Eq. (4). The congruent sublimation curve is given according to Goldfinger and Jeunehomme (6).

TABLE I
HOMOGENEITY RANGE OF CADMIUM TELLURIDE

$T(K)$	$P(kPa)$	X_S (at.% Te)	X_V (at.% Te)
Cd-saturated CdTe			
697.2	0.48	50.0002 ± 0.0002	0
819.6	4.46	50.0001 ± 0.0001	0
864.1	9.09	49.9990 ± 0.0001	0
871.3	10.18	49.9983 ± 0.0006	0
900.8	15.87	49.9990 ± 0.0001	0
939.7	27.87	49.9994 ± 0.0002	0
969.4	42.17	49.9991 ± 0.0002	0
992.0	57.26	49.9967 ± 0.0003	0
Te-saturated CdTe			
945.5	2.33	50.0006 ± 0.0001	99.9
1016.6	5.66	50.0036 ± 0.0001	99.9
1046.9	7.88	50.0055 ± 0.0004	99.9
1076.0	10.35	50.0073 ± 0.0001	99.8
1094.1	12.04	50.0092 ± 0.0003	99.8
1103.3	12.98	50.0098 ± 0.0001	99.7
1121.0	14.78	50.0138 ± 0.0007	99.6
1243.1	21.29	50.0087 ± 0.0008	96.5
1282.2	19.72	50.0050 ± 0.0010	96.0
1285.5	19.51	50.0047 ± 0.0015	90.8
1301.0	18.38	50.0044 ± 0.0030	85.6
1312.0	17.47	50.0038 ± 0.0040	77.7
1359.4	73.20	50.0034 ± 0.0006	2.0
1361.8	87.22	50.0013 ± 0.0004	0.8

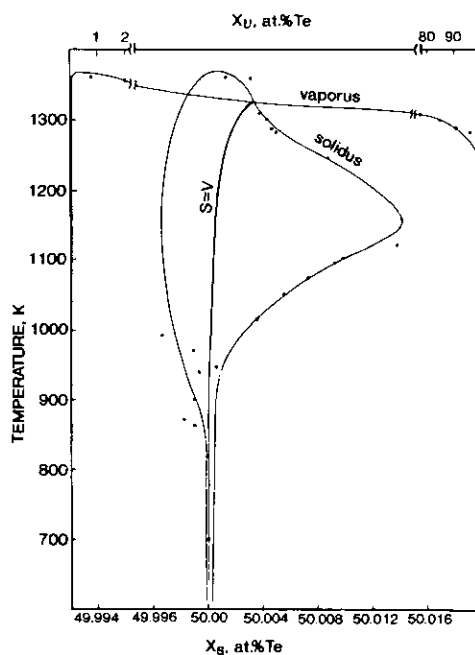


FIG. 1. T - X projection of the solidus and vaporus surfaces. The solid line is a best fit of the experimental results.

Partial Thermodynamic Functions

To calculate the partial vapor pressures of Cd and Te_2 for fixed X_S 's, the point solutions of Eqs. (1)–(11) for each vapor pressure curve were represented by the best-fit polynomials

$$\log P(i) = f_i(T) \quad (i = \text{Cd or } Te_2) \quad (14)$$

$$T = T(X_S). \quad (15)$$

Approximation procedure, standard for this laboratory (9), was used for the purpose. For an assumed X_S the corresponding temperature can be calculated from Eq. (15), and then $P(\text{Cd})$ and $P(\text{Te}_2)$ are obtained from Eq. (14) for every vapor pressure curve. The resulting $P(i)$ - T files were best fitted in the usual form $\log P(i) = A(i) - B(i)/T$, $i = \text{Cd or } Te_2$. The temperature dependencies of the partial vapor pressures are given in

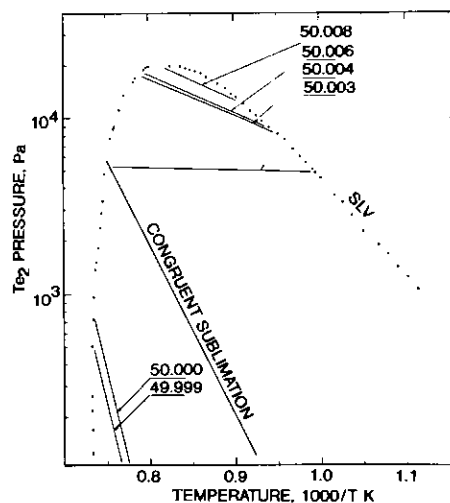


FIG. 2. $P(\text{Te}_2)$ - T projection of the single-phase volume of CdTe. The isopleths (in at.% Te) are drawn according to Table II and Fig. 1. The congruent sublimation curve is taken from Goldfinger (6).

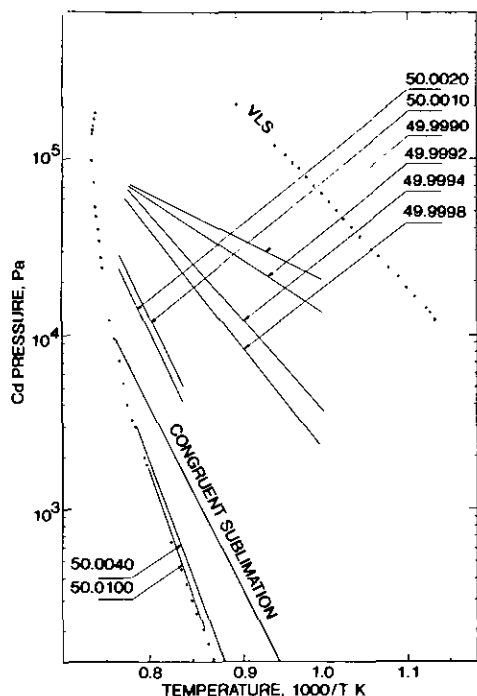


Fig. 3. $P(\text{Cd})$ - T projection of the single-phase volume of CdTe. The isopleths are in at.% Te.

Table II separately for solid CdTe in equilibrium with Cd-rich and Te-rich vapors (VS and SV equilibria, respectively). It can be seen that the Te-side surface of the solidus is in the $X_S > 50.004$ at.% Te region, while the Cd side spans $X_S = 49.999$ – 50.002 at.% Te and crosses the stoichiometric plane $X = 50$ at.%. Another characteristic feature of the sublimation region of CdTe reflected in Table II is that, in spite of a small X_S step (2×10^{-4} at.%), no X_S for which $B(\text{Cd}) = B(\text{Te}_2)$ was found. This means that no constant congruent sublimation composition of CdTe exists. As can be seen in Table II, these vapor pressure coefficients approach each other at $T > 1150$ K for $X_S = 50.001$ – 50.002 at.% Te, although $B(\text{Cd})$ in this region is slightly greater than $B(\text{Te}_2)$, implying that the congruently subliming composition X^{cs} gradually shifts from Cd to Te with increasing temperature. The last

row of Table II was calculated from mass-spectrometric data (6) for congruent sublimation of CdTe at low temperatures.

A standard thermodynamic procedure was used to calculate the partial molar enthalpies and entropies from the partial vapor pressures. Tabulated saturated vapor pressures of pure liquid Cd and Te (reference states) were taken from (5, 10). The results are also shown in Table II. The partial molar functions are independent of the composition of the solid for $X_S = 50.004$ – 50.01 at.% Te (equilibrium SV) and 50.0008 – 50.002 at.% Te (in VS) within the uncertainties, typical for the vapor pressure method, $\pm(4$ – $8)$ kJ/mole. A rigorous estimate of the uncertainties associated with the values in Table II proved to be rather difficult because a repeated best-fit procedure was used in these calculations.

Discussion

The total vapor pressure measurements at high temperatures resulted in two sets of scanning points, $\{P, T, X_s\}$ and $\{P, T, X_v\}$. From these the conjugated solidus and vapor surfaces were reconstructed in the P - T - X phase space. This procedure, known as the vapor pressure scanning of the solidus (9), proved to be sensitive enough to investigate deviations from stoichiometry as small as 10^{-3} to 10^{-4} at.% directly at high temperatures.

Since the compositional region of stability for CdTe is quite narrow (see Table I), special attention should be given to the uncertainties, δX_S , associated with the composition of the solid, X_S , obtained by this method. Three main sources contribute to these uncertainties: (1) experimental errors of measuring the vapor pressure, temperature, reaction volume, and initial masses; (2) uncertainties in thermodynamic functions of tellurium species; (3) the assumption that $\Delta G_T^\circ = \text{const.}$ at $T = \text{const.}$ within the single-phase region of CdTe. All of these

TABLE II
 PARTIAL PRESSURES, $\log P(i)(\text{Pa}) = A(i) - B(i)/T$, PARTIAL MOLAR ENTHALPIES (kJ/mole),
 AND ENTROPIES (J/mole · K)

$X_S(\% \text{Te})$	$A(\text{Cd})$	$10^3 B(\text{Cd})$	$H_m(\text{Cd})$	$S_m(\text{Cd})$	$A(\text{Te}_2)$	$10^3 B(\text{Te}_2)$	$H_m(\text{Te})$	$S_m(\text{Te})$
Equilibrium SV								
50.004	14.4 ± 0.1	13.9 ± 0.1	164.5	81.0	5.8 ± 0.1	2.0 ± 0.2	-38.1	-37.4
50.005	14.2 ± 0.1	13.7 ± 0.1	160.1	77.1	6.2 ± 0.1	2.4 ± 0.1	-34.1	-33.6
50.006	14.2 ± 0.1	13.7 ± 0.1	160.3	77.8	6.2 ± 0.1	2.4 ± 0.1	-34.1	-34.0
50.007	14.2 ± 0.1	13.7 ± 0.1	160.3	77.3	6.2 ± 0.1	2.4 ± 0.1	-34.1	-33.2
50.008	14.2 ± 0.1	13.7 ± 0.1	160.8	77.2	6.1 ± 0.2	2.2 ± 0.2	-35.9	-34.7
50.009	14.3 ± 0.1	13.8 ± 0.2	162.2	79.2	6.0 ± 0.1	2.1 ± 0.1	-36.9	-35.8
50.010	14.1 ± 0.3	13.7 ± 0.4	160.3	76.5	6.3 ± 0.6	2.4 ± 0.7	-34.1	-32.8
Equilibrium VS								
49.9990	6.4 ± 1.1	2.0 ± 1.1	-63.0	-72.0	21.9 ± 2.4	25.8 ± 2.4	190.3	116.6
49.9992	7.3 ± 2.0	3.1 ± 2.2	-42.0	-54.8	20.0 ± 4.0	23.5 ± 4.5	167.9	98.3
49.9994	9.4 ± 1.8	5.8 ± 2.1	9.4	-14.0	15.7 ± 3.6	18.1 ± 4.2	116.0	57.1
49.9996	10.0 ± 2.8	6.7 ± 3.3	25.7	-2.3	14.4 ± 5.3	16.3 ± 6.6	99.2	45.0
49.9998	9.6 ± 2.7	6.3 ± 3.3	18.5	-9.4	15.2 ± 5.4	17.1 ± 6.6	106.5	52.1
50.0000	9.4 ± 3.2	6.1 ± 3.7	14.2	-13.2	15.6 ± 7.5	17.5 ± 8.1	110.8	56.0
50.0002	9.3 ± 0.1	5.9 ± 0.1	10.1	-15.6	15.9 ± 0.1	18.1 ± 0.1	116.0	59.3
50.0004	10.8 ± 0.7	8.0 ± 0.8	50.3	11.9	13.0 ± 1.4	13.9 ± 1.7	75.8	31.8
50.0006	11.9 ± 1.4	9.6 ± 1.7	81.6	34.5	10.6 ± 2.9	10.6 ± 2.9	44.1	8.8
50.0008	12.3 ± 2.3	10.1 ± 2.8	91.1	40.6	10.0 ± 4.6	9.6 ± 5.5	13.5	2.6
50.0010	12.1 ± 0.9	10.0 ± 1.1	88.6	37.8	10.3 ± 1.7	9.8 ± 2.1	36.5	5.4
50.0012	12.0 ± 0.5	9.9 ± 0.7	87.2	36.1	10.5 ± 1.1	9.9 ± 1.3	38.2	7.0
50.0014	12.0 ± 0.5	9.9 ± 0.7	86.8	35.9	10.5 ± 1.1	10.0 ± 1.3	38.7	7.4
50.0016	12.0 ± 0.3	10.0 ± 0.4	88.7	36.8	10.4 ± 0.7	9.8 ± 0.8	36.7	6.2
50.0018	12.0 ± 0.5	9.9 ± 0.6	87.9	35.2	10.5 ± 1.0	9.8 ± 1.2	37.2	7.6
50.0020	11.9 ± 0.6	10.0 ± 0.7	88.8	34.9	10.5 ± 1.1	9.7 ± 1.4	36.2	7.9
(6) ^a	11.40	9.76	84.85	24.3	11.099	9.76	36.4	13.61

^a Congruent sublimation according to Goldfinger (6).

factors influence δX_S in different ways, depending on the experimental conditions.

(1) The uncertainties in δX_S resulting from the experimental errors were readily calculated at every experimental point by applying the error accumulation law, since all the experimental errors were known. It was shown that the main source of the uncertainties was the precision of the balance (5×10^{-5} g in our experiments) which led to a typical δX_S value within $(1-5) \times 10^{-4}$ at.%. (2) It is difficult to estimate rigorously the thermodynamic functions of all the tellurium polymers Te_k (7). To avoid the need to do so, an additional set of X_S calculations

was made, with Te_2 as the only tellurium species (the thermodynamics of this molecule is the most reliable (7)). The result was that both Te_k and Te_2 models gave the same X_S values within the uncertainties caused by the experimental errors. (3) The influence of the $\Delta G_T^\circ = \text{const.}$ assumption on the calculated X_S 's was checked by fluctuating the ΔG_T° values within $\pm(2-4)$ kJ/mole, the expected variation of ΔG_T° within the homogeneity range of CdTe (11). It was shown that in the VS equilibrium, with the vapor made up of almost pure Cd ($X_V \cong 10^{-4}$ at.% Te), this influence was undetectable. For the SV equilibrium (Te nonstoichiometry) at $T < 1250$ K the variations of X_S

were negligible compared to the δX_S associated with the experimental errors. At higher temperatures (1250–1350 K) the $\Delta G_T^0 = \text{const.}$ assumption influenced the calculated X_S 's quite noticeably, up to 3×10^{-3} at.% Te in some experiments. All the X_S values in Table I are listed with the calculated uncertainties which incorporated all the above-mentioned contributions.

As an independent check of the results, X_S was also determined at several (P, T) points using the intersection method devised in this laboratory (9). In this method the composition of the solid CdTe, X_S , is calculated from X_S (at.% Te)

$$= \frac{N_{\text{Te1}}V_2 - N_{\text{Te2}}V_1}{(N_{\text{Cd1}} + N_{\text{Te1}})V_2 - (N_{\text{Cd2}} + N_{\text{Te2}})V_1} \cdot 100\% \quad (16)$$

at the intersection point of two vapor pressure curves, 1 and 2, and is independent of the composition of the vapor. In Eq. (16) N_{Cd1} , N_{Te1} , V_1 and N_{Cd2} , N_{Te2} , V_2 are the initial masses and reaction volumes which characterize the two intersecting vapor pressure curves. It was proved that the X_S values obtained by this method were the same as those calculated from the $\Delta G_T^0 = \text{const.}$ model to within $\leq 4 \times 10^{-4}$ at.%.

Estimation of the uncertainties of the vapor composition X_V is reasonable only for the SV equilibrium, since in VS the vapor is almost pure Cd (see Table I). Because of uncertainties in the thermodynamics of Te_k polymers (7), δX_V 's were estimated by comparing two models of the vapors, Te_2 only and Te_k , $k = 1$ to 7. The resulting δX_V values were within 0.5 at.% at $T < 1280$ K, whereas at higher temperatures the uncertainties of δX_V rose to $\pm(1-3)$ at.%.

Special attention should be given to the last two rows of the Te solubility section of Table I. These two vapor pressure curves (for initial samples 49.94 and 49.95 at.% Te) went through the VS region and

intersected the steeply ascending portion of the three-phase curve at 1359.4 and 1361.8 K, respectively. According to our previous publication (8), this is the VSL branch of the three-phase curve, with the liquid enriched in Te compared to the solid. This means that the intersection points correspond to the $\text{VS} \Rightarrow \text{VSL}$ phase transition; i.e., the compositional sequence of the vapor and solid phases in these equilibria remained unchanged. This proves that these two curves did not meet the congruent sublimation curve $S = V$. Therefore, the maximum congruent sublimation point of CdTe is lower than 1359 K, and corresponds to the composition $X^{\text{cs}} > 50.0034$ at.% Te. The actual maximum congruent sublimation temperature was found as a point of tangency of the SLV and $S = V$ curves. The former was taken from (8) while the latter was calculated from the thermodynamic functions of CdTe(s) and all the gaseous species. The congruent sublimation point, calculated in this way, is $T_{\text{Max}}^{\text{cs}} = 1324$ K, which is 41 K lower than the maximum melting point of CdTe (11). The $T-X$ projection of the congruent sublimation curve is shown in Fig. 1, while the $P(\text{Cd})-T$ and $P(\text{Te}_2)-T$ projections are given in Figs. 2 and 3.

It should be stressed that under the conditions outlined in the last two rows of Table I, the crystal with superstoichiometric tellurium is in three-phase equilibrium with Te-rich melt and the vapor which is virtually pure Cd (0.8 to 2.0 at.% Te). This also implies that at the maximum melting point CdTe is in equilibrium with the vapor $X_V < 0.8$ at.% Te. This compares quite well with the $X_V \cong 2$ at.% Te at T_{Max} reported by Brebrick (11). Also in agreement with (11) (to within the $\pm 10\%$ confidence interval adopted by Brebrick) are the Te_2 partial pressures in SLV equilibrium (Fig. 2) up to about 1200 K.

The homogeneity range of CdTe listed in Table I differs considerably from that ob-

tained from Hall effect measurements (12), especially on the Te side where maximum solubility is 1 to 2 orders of magnitude greater than that calculated from the Hall data (12). This can be attributed either to nonequilibrium Hall data or to electrical inactivity of the native defects in Te-saturated CdTe.

References

1. W. ALBERS, in "Current Topics in Materials Science" (E. Kaldis, Ed.) Vol. 10, North-Holland, Amsterdam (1982).
2. V. P. ZLOMANOV AND A. V. NOVOSYOLOVA, "P-T-X Phase Diagrams of the Systems Metal-Chalcogen," Nauka, Moscow (1987).
3. F. A. KROGER, "The Chemistry of Imperfect Crystals," North-Holland, Amsterdam (1964).
4. V. B. LAZAREV, J. H. GREENBERG, AND B. A. POPOVKIN, in "Current Topics in Materials Science" (E. Kaldis, Ed.), Vol. 1. p. 657, North-Holland, Amsterdam (1978).
5. R. HULTGREN, R. L. ORR, P. D. ANDERSON, AND K. K. KELLEY, "Selected Values of Thermodynamic Properties of Metals and Alloys," Wiley, New York (1963).
6. P. GOLDFINGER AND M. JEUNEHOMME, *Trans. Faraday Soc.* **59**, 2851 (1963).
7. "Thermodynamic Data Base IVTANTERMO," Academy of Science, USSR.
8. J. H. GREENBERG, V. N. GUSKOV, V. B. LAZAREV, A. A. KOTLIAR, AND A. V. NAMM, *Dokl. Akad. Nauk SSSR [Proc. Acad. Sci. USSR, Phys. Chem.]* **305**(5), 1152 (1989).
9. J. H. GREENBERG AND V. B. LAZAREV, in "Current Topics in Materials Science" (E. Kaldis, Ed.), Vol. 12, p. 119, North-Holland, Amsterdam (1985).
10. L. S. BROOKS, *J. Am. Chem. Soc.* **74**, 227 (1952).
11. R. F. BREBRICK, *J. Electrochem. Soc.* **118**, 2014 (1971).
12. F. T. J. SMITH, *Metallurg. Trans.* **1**, 617 (1970)