

## The Defect Structure of CdTe: Self-Diffusion Data\*

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Cadmium and Te tracer self-diffusion was studied for pure and indium-doped CdTe. Analysis of the results leads to a point defect model in which imperfections with various charges play a role. Expressions for the tracer diffusion coefficients by various mechanisms and for the diffusion coefficients of individual point defects are derived.

### Introduction

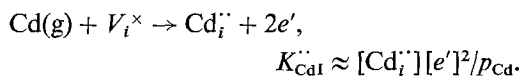
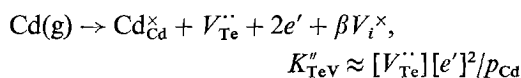
Self-diffusion and its dependence on component activities provides us with a valuable tool to establish the defect structure of crystalline compounds (1). It has been used with success with various compounds; we may mention in particular, work on ZnO (2), CdO (3), and CdS (4). For CdTe, de Nobel (5), in a preliminary experiment, found that cadmium self-diffusion increases with increasing  $p_{Cd}$ . Cadmium self-diffusion studies by Whelan and Shaw (6) and Borsenberger and Stevenson (7), however, indicate that  $D_{Cd}^*$ , the Cd-tracer diffusion coefficient, is independent of  $p_{Cd}$ . The tracer diffusion coefficient  $D_{Cd}^*$  is related to the site fraction of point defects involved in the diffusion process,  $[j]$ , by

$$D_{Cd}^* = \sum_j f_j D_j [j], \quad (1)$$

where  $f_j$  are correlation coefficients and  $D_j$  the diffusion constants of the defects  $j$ . The sum sign is used when  $D_{Cd}^*$  has contributions by various defects. If only one defect contributes, a  $D_{Cd}^*$  independent of  $p_{Cd}$  as observed for CdTe indicates that the concentration of the defects involved is independent of  $p_{Cd}$ . It was attempted to explain this independence by assuming a disorder structure

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dominated by native atomic disorder, either Schottky disorder with  $[V_{Cd}^{\cdot\cdot}] \approx [V_{Te}^{\cdot\cdot}] \approx \sqrt{K_S''}$ , or Frenkel disorder of Cd with  $[Cd_i^{\cdot\cdot}] \approx [V_{Cd}^{\cdot\cdot}] \approx \sqrt{K_F''}$ ,  $K_S''$  and  $K_F''$  being the constants of Schottky and Frenkel disorder. However, this explanation conflicts with the results of Hall effect measurements by Smith (8) and ourselves (9) at high  $p_{Cd}$ , which indicate that doubly charged native donors,  $D_n^{\cdot\cdot}$  are formed. These consist of  $V_{Te}^{\cdot\cdot}$  and  $Cd_i^{\cdot\cdot}$ , formed by the reactions



Here  $\beta$  is the number of  $V_i^{\times}$  present per molecule of CdTe.

$$[D_n^{\cdot\cdot}] = [V_{Te}^{\cdot\cdot}] + [Cd_i^{\cdot\cdot}] =$$

$$(p_{Cd}/[e']^2)(K_{TeV}'' + K_{CdI}'')$$

or, by introducing a formation constant  $K_{D_n}^{\cdot\cdot}$  for  $D_n^{\cdot\cdot}$ ,

$$K_{D_n}^{\cdot\cdot} = [D_n^{\cdot\cdot}][e']^2/p_{Cd} = K_{TeV}'' + K_{CdI}''.$$

A model dominated by Schottky or Frenkel disorder would make  $[V_{Te}^{\cdot\cdot}]$  and  $[Cd_i^{\cdot\cdot}]$  independent of  $p_{Cd}$ , leading to  $[e'] \propto p_{Cd}^{1/2}$  and not  $p_{Cd}^{1/3}$  as observed. A  $D_{Cd}^*$  independent of  $p_{Cd}$  can be explained by assuming diffusion by a ring mechanism (10). This can be visualized

either as a mechanism not involving defects or as a mechanism in which the defects involved represent the transition state of the diffusion process. For a two-member ring this could be  $(V_{Cd}Cd_i)^{\times}$ , the concentration of which is independent of  $p_{Cd}$ . In the former case the activation energy of  $D_{Cd}$  is that of the ring process; in the latter it is that of defect formation, with  $D(V_{Cd}Cd_i)$  independent of temperature. Diffusion involving an associate  $(V_{Cd}V_{Te})^{\times}$ , the concentration of which would also be independent of  $p_{Cd}$ , would lead to a tellurium diffusion equal to or larger than the Cd diffusion—contrary to what has been observed (7). Therefore, this species cannot be invoked to explain the observed pressure independence.

In CdS, Cd self-diffusion has been found to be strongly  $p_{Cd}$  dependent with singly ionized  $Cd_i^+$  the dominant carrier of Cd at high  $p_{Cd}$ , and  $V_{Cd}''$  the dominant carrier at low  $p_{Cd}$  (4). In CdSe the situation is similar; the only difference is that now both singly and doubly ionized  $Cd_i^+$  and  $Cd_i^{2+}$  contribute at high  $p_{Cd}$  (11). In view of this it is tempting to assume that, also in CdTe, charged single species are involved and the apparent independence of  $p_{Cd}$  comes about by the superposition of contributions from different defects with opposite  $p_{Cd}$  dependencies. An indication that this may indeed be the case is found in the work of Borsenberger and Stevenson (7), who found that doping with Al (a donor) gives rise to a markedly increased  $D_{Cd}^*$  with a lower activation energy; this effect may be explained by the increase of the concentration of negatively charged Cd-transporting species such as  $V_{Cd}'$  or  $V_{Cd}''$ .

The work reported in the present paper was undertaken to investigate this possibility and to see whether a defect model can be found that explains all experimental data presently available. As we shall see, this was the case.

The experiments to be reported on are the following: (i) Cd self-diffusion studies of pure and indium (= donor)-doped CdTe as  $f(p_{Cd}, T)$ ; (ii) Te self-diffusion studies in pure CdTe. Tellurium diffusion at low  $p_{Cd}$  is known to be proportional to  $p_{Cd}^{-1}$ , as is typical for diffusion involving uncharged  $Te_i^{\times}$  (7, 12). Similar

behavior has been found for chalcogen self-diffusion in CdS, CdSe, ZnTe, PbS, PbSe, PbTe and therefore can be accepted without further study. The behavior at high  $p_{Cd}$  is less well established, however. We have limited our Te diffusion studies to this range.

## Experimental

### Sample Preparation

Single crystals of undoped CdTe and of CdTe- $10^{17}$  In  $cm^{-3}$  were put at our disposal by Dr. K. Zanio of Hughes Aircraft Research Laboratory, Malibu, CA. Spectrographic analysis showed that impurities, if present, are below the detection limits. Samples doped with  $2.7 \times 10^{17}$  In  $cm^{-3}$  were made from the lightly doped crystal by indiffusion of indium (see (9) for details). A crystal of CdTe- $3.6 \times 10^{18}$  In  $cm^{-3}$  was made by subliming CdTe with the addition of some indium at  $p_{Cd} = 10^{-2}$  atm. Samples of  $1 \times 4 \times 4$  mm were cut from the boules with the aid of a wiresaw; they were washed with trichloroethylene and etched for 100 min in a solution of 10 wt% bromine in methanol. Samples from the same boules were used for Hall measurements reported in the first paper (9).

In Figs. 2-4 the undoped samples will be referred to as  $U$ , the weakly doped ones as  $D_1$ , and the heavily doped ones as  $D_2$ .

### Preparation of Cd and Te Tracer Sources for Diffusion

Cadmium tracer ( $Cd^{109}$ ,  $\gamma$ , 0.09 MeV) was received from New England Nuclear Corp. as  $CdCl_2$  in 0.5 N HCl in amounts of 1 mCi. The initial solution containing all the activity with 0.4 mg Cd in a volume of 0.1-0.2 ml was diluted with deionized water to 2 ml. Two drops of this solution were transferred to a small quartz tube (4-mm i.d., 3.2 cm long) and two drops of concentrated  $HNO_3$  were added to convert  $CdCl_2$  to  $Cd(NO_3)_2$ . The solution was dried by heating to  $95^\circ C$  for several hours. Preliminary diffusion experiments revealed that reliable results were only obtained if oxygen is absent. Any oxygen present acts as a transport agent during the diffusion run and causes sublimation of the samples with continuous removal of its surface layer, which thus

upsets the tracer penetration profile. Therefore, the  $\text{Cd}(\text{NO}_3)_2$  was reduced to metallic Cd by a stream of dry hydrogen at  $\sim 280^\circ\text{C}$  (for a detailed description of the procedure followed, see (13)). The small quartz tube with Cd tracer was introduced into the diffusion apparatus containing the crystal sample.

Tellurium tracer,  $\text{Te}^*$  ( $\text{Te}^{123}$ ,  $\gamma$ , 0.0886 MeV) was received from Union Carbide Corp. as  $\text{TeCl}_4$  in HCl in batches of 1 mCi in a solution volume of 1.5 ml. Three or 4 drops of this solution, containing about 50  $\mu\text{Ci}$  were transferred into a U-shaped tube and diluted with 6 drops of deionized water. Cleaned graphite rods were inserted into the two openings of the U-tube, a voltage was applied, and  $\text{Te}^*$  was deposited on the graphite cathode by electrolysis at a potential of 0.63–0.65 V. The tracer-loaded cathode was rinsed with water, and dried, first with filter paper and then *in vacuo*.

#### Diffusion Experiments

$\text{Cd}^*$  and  $\text{Te}^*$  tracer self-diffusion experiments in pure and donor-doped CdTe were carried out isothermally at 700, 800, and  $900^\circ\text{C}$ , respectively, under well-defined Cd pressures, chosen to fall inside the stability region of CdTe as determined by de Nobel (5) and Lorenz (14) but sufficiently removed from the minimum pressure to avoid sublimation. Although samples were not previously equilibrated under the conditions used in the experiments, the time involved in establishing equilibrium with the atmosphere by chemical diffusion is so small relative to the tracer penetration time that the experiment may be considered to be isoconcentrational as far as the defects are concerned.

For  $\text{Cd}^*$  tracer experiments the small quartz tube with the tracer prepared as described earlier was introduced into a wider quartz tube together with a cleaned crystal and 20 mg of Cd or Te. Then the tube was evacuated and sealed. The Cd used was etched with 1 vol  $\text{HNO}_3$  in 3 vol  $\text{H}_2\text{O}$ . The Te was etched with aqua regia. For the diffusion experiment the tube was placed in a two-temperature zone furnace with the crystal at the highest temperature.

For  $\text{Te}^*$  diffusion experiments the same

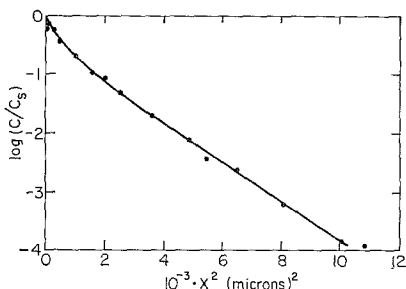


FIG. 1. Experimental tracer penetration profile (points) and theoretical complementary error function (line) showing the type of agreement that is usually obtained.  $Dt = 1.37 \times 10^{-5} \text{ cm}^2$ .

procedure was followed with  $\text{Te}^*$  instead of  $\text{Cd}^*$ . Under these conditions, constant surface activities are maintained, as witnessed by satisfactory representation of tracer penetration profiles by a complementary error function solution of the diffusion equation

$$c^*(x, t) = c_0^* \text{erfc}(x^2/4D^*t)^{1/2},$$

where  $c_0^*$  is the tracer concentration at the surface,  $x$  the distance from the surface, and  $t$  time. Figure 1 shows a representative example. Sectioning was done as described in (4).

## Experimental Results

### Diffusion Constants

Cadmium tracer diffusion constants for pure and doped CdTe as  $f(p_{\text{Cd}})$ , measured in our experiments at 700, 800, and  $900^\circ\text{C}$ , are shown in Figs. 2–4. Tellurium tracer diffusion constants, measured for pure CdTe at 700, 800, and  $900^\circ\text{C}$ , are shown in Fig. 5. The data are reproducible within a deviation of  $\pm 10\%$ , which can be attributed to errors in the various steps of the measurements.

It is seen that the Cd tracer diffusion constants  $D_{\text{Cd}}^*$  for undoped crystals are practically independent of  $p_{\text{Cd}}$  for Cd pressures equal to or smaller than one-tenth of the Cd saturation pressure. At high Cd pressures there is a small but significant increase of  $D_{\text{Cd}}^*$  with  $p_{\text{Cd}}$  at 800 and  $900^\circ\text{C}$ :  $D_{\text{Cd}}^* \propto p_{\text{Cd}}^n$ , with  $n \approx \frac{1}{3}$ . At  $700^\circ\text{C}$  the increase is smaller.  $D_{\text{Cd}}^*$  for crystals doped with  $2.7 \times 10^{17} \text{ In cm}^{-3}$  does not differ appreciably from those of the

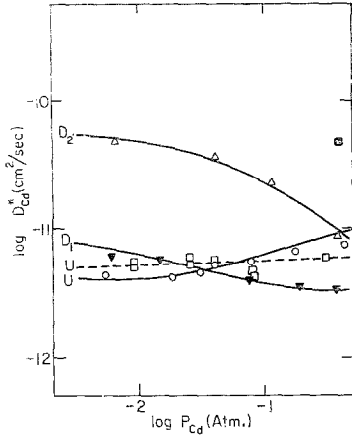


FIG. 2. Variation of  $D_{Cd}$  with  $p_{Cd}$  for undoped CdTe ( $U$ ), CdTe- $2.7 \times 10^{17}$  In  $cm^{-3}$  ( $U_1$ ), and CdTe- $3.6 \times 10^{18}$  In  $cm^{-3}$  ( $D_2$ ) at  $700^\circ C$ . The dashed line and the square solid points represent results by Borsenberger and Stevenson (7) for undoped CdTe and CdTe with  $5 \times 10^{17}$  Al  $cm^{-3}$ . Experiment and theory:  $\circ$ , —,  $U$ ;  $\square$ , —,  $U$  (7);  $\nabla$ , —,  $D_1$ ;  $\Delta$ , —,  $D_2$ . Experiment:  $\blacksquare$ , CdTe- $5 \times 10^{17}$  Al  $cm^{-3}$  (7).

undoped crystals at low  $p_{Cd}$ . At high  $p_{Cd}$ ,  $D_{Cd}^*$  is somewhat smaller than for undoped crystals. In both regions the  $p_{Cd}$  dependence is weak. For crystals doped with  $3.6 \times 10^{18}$  In  $cm^{-3}$ ,  $D_{Cd}^*$  is markedly increased at low  $p_{Cd}$  and weakly increased at high  $p_{Cd}$ ;  $D_{Cd}^*$  decreases monotonically with increasing  $p_{Cd}$

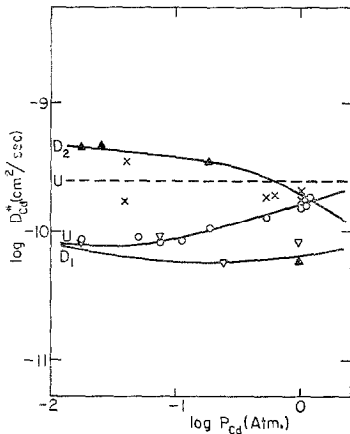


FIG. 3. Variation of  $D_{Cd}^*$  with  $p_{Cd}$  for undoped and indium-doped CdTe at  $800^\circ C$ . Experiment and theory:  $\circ$ , —,  $U$ ;  $\times$ , —,  $U$  (6);  $\nabla$ , —,  $D_1$ ;  $\Delta$ , —,  $D_2$ .

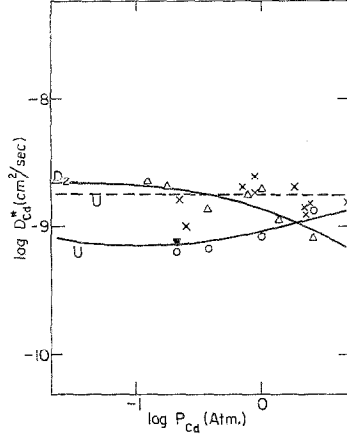


FIG. 4. Variation of  $D_{Cd}^*$  with  $p_{Cd}$  for undoped and indium-doped CdTe at  $900^\circ C$ . Experiment and theory:  $\circ$ , —,  $U$ ;  $\times$ , —,  $U$  (6);  $\Delta$ , —,  $D_2$ . Experiment:  $\nabla$ ,  $D_1$ .

over the whole range. If we write  $D_{Cd}^* \propto p_{Cd}^s$ ,  $0 < s < 1$ . At low  $p_{Cd}$  and  $T = 700^\circ C$ ,  $D_{Cd}^*$  in the strongly doped crystal is about eight times that for the weakly doped crystal, while the ratio of the indium concentrations is 13.3. This factor is smaller at higher temperatures. The dependence of  $D_{Cd}^*$  at  $700^\circ C$  on the indium concentration at high and low  $p_{Cd}$  is shown in Fig. 6. At high  $p_{Cd}$  an initial decrease due to indium doping at low con-

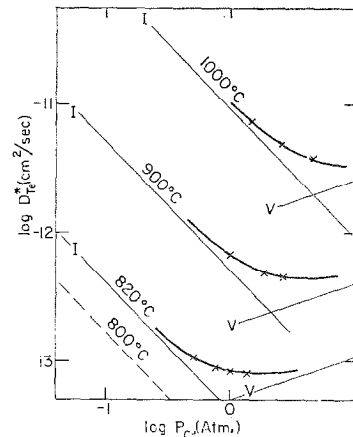


FIG. 5. Variation of  $D_{Te}^*$  with  $p_{Cd}$  for undoped CdTe at 800, 900, and  $700^\circ C$ . The dashed  $800^\circ C$  line is due to Woodbury and Hall (12) and Borsenberger and Stevenson (7). I and V indicate diffusion by an interstitial and vacancy mechanism, respectively.

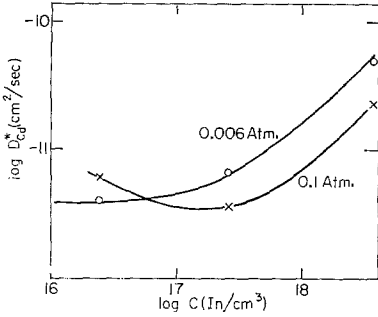


FIG. 6. Variation of  $D_{\text{Cd}}^*$  with indium concentration at two  $p_{\text{Cd}}$ 's at  $700^\circ\text{C}$ .

centration is followed by an increase at high indium concentration. At low  $p_{\text{Cd}}$  there is an increase throughout—weak at low, stronger at high indium concentrations. An increase by doping with donors was also observed by Borsenberger and Stevenson (7). These effects indicate that, in undoped CdTe, Cd is transported mainly by a positive species at high  $p_{\text{Cd}}$  but by a negative species at low  $p_{\text{Cd}}$ .

Since tellurium diffusion is known to be proportional to  $p_{\text{Cd}}^{-1}$  at low  $p_{\text{Cd}}$  (12), we have restricted our measurements to high  $p_{\text{Cd}}$ 's. As seen in Fig. 5,  $D_{\text{Te}}^*$  at high  $p_{\text{Cd}}$  is almost independent of  $p_{\text{Cd}}$ . This indicates a transition from a low  $p_{\text{Cd}}$  mechanism with  $D_{\text{Te}}^* \propto p_{\text{Cd}}^2$  with  $\alpha = \alpha_1 = -1$  to a high  $p_{\text{Cd}}$  mechanism with  $\alpha = \alpha_2 > 0$ . It is possible to represent the data with  $\alpha = \alpha_2 = \frac{1}{3}$ . The low  $p_{\text{Cd}}$  curves have been drawn to fit data by Woodbury and Hall (12) and Borsenberger and Stevenson (7). Figures 2–5 show also experimental results for  $D_{\text{Cd}}^*$  and  $D_{\text{Te}}^*$  due to other workers. Our data are close to those of Borsenberger and Stevenson (7), but they deviate somewhat from those of Whelan and Shaw (6), whose values are approximately two times ours.

## Discussion

Our results indicate that charged defects contribute to both  $D_{\text{Cd}}^*$  and  $D_{\text{Te}}^*$ . As we saw in the Introduction, the diffusion coefficients are proportional to the defect concentrations with the diffusion constants of the individual defects involved and the corresponding correlation coefficients as multipliers. In isotherms the defect diffusion constants are constant, and therefore the variations of the

tracer diffusion constants with  $p_{\text{Cd}}$  are directly related to the variations of the concentrations of defects. These in turn are uniquely determined by the values of the equilibrium constants of the reactions by which the various defects are formed, as described by defect chemistry. Once the defect concentrations at one  $p_{\text{Cd}}$  and dopant concentration are known, the values of the equilibrium constants are fixed, and the concentrations of the defects at all other cadmium pressures and dopant concentrations are also fixed and can be calculated by the methods of defect chemistry. We therefore know in what way the concentrations of individual defects will vary with variation of  $p_{\text{Cd}}$  and/or dopant concentration. This makes it possible to determine the contributions by the individual defects to  $D_{\text{Cd}}^*$  and  $D_{\text{Te}}^*$  by analyzing the shape of  $D_{\text{Cd}}^*$  and  $D_{\text{Te}}^*$  isotherms as a function of  $p_{\text{Cd}}$  or dopant concentration. In carrying out the analysis (which is described in greater detail in (13)) we are led initially by predictions based on appropriate approximations made to the neutrality condition and the dopant balance equation (Brouwer's approximation (15)), which give typical pressure dependences for the individual defects. Finally, however, the complete neutrality condition and balance equation are used. In order to start the analysis we must have some idea about the types of defects to be expected. Also, we preferably start in a range in which Brouwer's approximation is close to the exact solution. This is the case with both undoped and doped CdTe at high  $p_{\text{Cd}}$ . In undoped CdTe under these conditions  $[D_n^{\cdot\cdot}] \approx 2[e'] \propto p_{\text{Cd}}^{1/3}$ ; in indium-doped CdTe it is  $[\text{In}_{\text{Cd}}^{\cdot}] \approx [e']$ . Since the two components of  $D_n^{\cdot\cdot}$ ,  $\text{Cd}_i^{\cdot}$  and  $V_{\text{Te}}^{\cdot}$ , show the same dependence on  $p_{\text{Cd}}$ , the ratio in which they contribute cannot be determined on this basis. The same applies to native acceptors becoming important at low  $p_{\text{Cd}}$ ,  $A_n'$  consisting of  $V_{\text{Cd}}'$  and  $\text{Te}_i'$  and  $A_n''$  consisting of  $V_{\text{Cd}}''$  and  $\text{Te}_i''$ . As shown in (9) the relative contributions of these can be determined with the aid of semiconductor statistics on the basis of known positions of relevant electronic energy levels. On this basis it was established that  $[A_n''] \approx [V_{\text{Cd}}'']$ ,  $[V_{\text{Cd}}'] \approx [\text{Te}_i']$ .

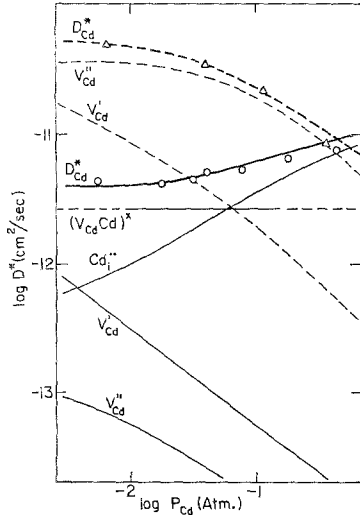


FIG. 7. Contributions by various mechanisms to the Cd tracer diffusion in undoped CdTe and CdTe- $3.6 \times 10^{18}$  In  $\text{cm}^{-3}$  at  $700^\circ\text{C}$  V as a function of  $p_{\text{Cd}}$ .  $\Delta$ , ---:  $3.6 \times 10^{18}$  In  $\text{cm}^{-3}$ ;  $\circ$ , —: undoped.

We can account for the shape of  $D_{\text{Cd}}^*$  isotherms for both undoped and doped CdTe if we assume that, at the point where  $[e'] \approx [h']$ ,  $[A_n']/[A_n''] \approx 8$  at  $700^\circ\text{C}$ , 5 at  $800^\circ\text{C}$ , and 2.8 at  $900^\circ\text{C}$ . However, this is only possible if we add a contribution by a pressure-independent ring mechanism assumed to involve  $(\text{Cd}_i \text{V}_{\text{Cd}})^x$ . This contribution has been

chosen in such a way that it follows an exponential dependence on  $T^{-1}$  as required by thermodynamics. The same applies to the contributions by  $A_n'$  and  $A_n''$ . Figure 7 shows the result of the analysis for undoped CdTe and CdTe- $3.6 \times 10^{18}$  In  $\text{cm}^{-3}$  at  $700^\circ\text{C}$ . The

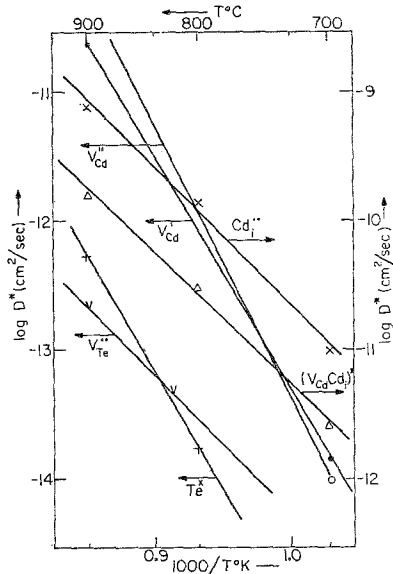


FIG. 8. Contributions by various mechanisms to the tracer diffusion  $D_{\text{Cd}}^*$  and  $D_{\text{Te}}^*$  in undoped CdTe at  $p_{\text{Cd}} = 1$  atm as a function of temperature.

TABLE I  
CONTRIBUTIONS TO  $\text{Cd}^*$  AND  $\text{Te}^*$  DIFFUSION BY VARIOUS DEFECTS  
IN UNDOPED CdTe AT HIGH  $p_{\text{Cd}}$ :

$$D^* = D_0^* p_{\text{Cd}}^a \exp(-H^*/kT) \text{ (CM}^2 \text{ SEC}^{-1}\text{)}$$

$D^*$	$D_0^*$ ( $\text{cm}^2 \text{ sec}^{-1} \text{ atm}^{-a}$ )	$a$	$H^*$ (eV)
$D_{(\text{V}_{\text{Cd}} \text{Cd}_i)^x}^*$	$6.67 \times 10^{-2}$	0	2.01
$D_{\text{Cd}_i^+}^*$	0.95	$\frac{1}{3}$	2.11
$D_{\text{V}_{\text{Cd}}'}^*$	$7.1 \times 10^5$	$-\frac{2}{3}$	3.83
$D_{\text{V}_{\text{Cd}}}^*$	$3.33 \times 10^7$	$-\frac{1}{3}$	4.2
$D_{\text{V}_{\text{Te}}}^*$	$4.35 \times 10^{-4}$	$\frac{1}{3}$	2.11
$D_{\text{Te}_i^x}^*$	$2.75 \times 10^3$	-1	3.6
$D_{\text{Cd}}^*$ (total)	$3.26 \times 10^2$	—	2.67 (saturated $p_{\text{Cd}}$ ) <sup>b</sup>
$D_{\text{Cd}}^*$ (total)	$1.58 \times 10$	—	2.44 (saturated $p_{\text{Te}_2}$ ) <sup>b</sup>
$D_{\text{Te}}^*$	$1.66 \times 10^{-4}$	—	1.38 (saturated $p_{\text{Te}_2}$ ) <sup>b</sup>
$D_{\text{Te}}^*$	$8.54 \times 10^{-7}$	—	1.42 (saturated $p_{\text{Cd}}$ ) <sup>b</sup>

<sup>b</sup> Data according to (7)

TABLE II  
DEFECT DIFFUSION CONSTANTS,  $D$ , AND DEFECT FORMATION CONSTANTS,  
 $K$ , AS A FUNCTION OF  $T$ :

$$D = D_0 \exp(-H/kT) \text{ (CM}^2 \text{ SEC}^{-1}\text{) OR } K = K_0 \exp(-H/kT)$$

$D$	$D_0$ (cm <sup>2</sup> sec <sup>-1</sup> )	$H$ (eV)
$D_{Cd_i}^*/[D_n^{**}] = D_{Cd_i} [Cd_i']/[D_n^{**}]$	$2.63 \times 10^2$	1.49
$D_{V_{Cd}}^-$	$390/f_c$	1.63
$D_{V_{Cd}}^-$	$2.74 \times 10^3/f_c (1.37)^a$	1.85 (2) <sup>a</sup>
$D_{V_{Cd}}^-$ in CdS <sup>b</sup>	4.39	1.48
$D_{V_{Te}}^-$	$5.7 \times 10^{-2}/f_c$	1.42
$D_{V_S^{**}}$ in CdS <sup>b</sup>	$5.32 \times 10^{-4}/f_c$	1.32
$D_{Te_i^x}$	$2.04 \times 10^{-2}$	0.42 <sup>c</sup>
$D_{Cd_i^*}$	21.7	1.21

<sup>a</sup> Data according to (7).

<sup>b</sup> Data according to (4).

<sup>c</sup> Estimated for a  $Te_i'$  level at  $E_v + 0.15$  eV.

result for CdTe— $2.7 \times 10^{17}$  In cm<sup>-3</sup> (not shown) is equally good. Isotherms for other temperatures, synthesized in a similar way, are shown in Figs. 3 and 4. The tellurium tracer diffusion coefficient  $D_{Te}^*$  for undoped CdTe shown in Fig. 5 has contributions by  $Te_i^x$  (giving  $D_{Te}^* \propto p_{Cd}^{-1}$ ) and  $V_{Te}^{**}$  (giving  $D_{V_{Te}}^{**} \propto p_{Cd}^{1/3}$ ), with  $D_{Te}^* = D_{Te_i^x}^* + D_{V_{Te}}^{**}$ .

The individual contributions to  $D_{Cd}^*$  and  $D_{Cd}^*$  for undoped CdTe at various temperatures are shown in Fig. 8. Table I gives the parameters of  $D^*(p_{Cd}, T)$ .

In a previous paper, by using the ratios of  $[A_n']/[A_n'']$  derived in the present work, a defect model was presented which accounted in a satisfactory way both for high-temperature Hall data and the Hall data by de Nobel on cooled crystals. Using the constants determined there, we can calculate the concentrations of individual defects as a function of  $p_{Cd}$ ,  $T$ , and  $[In]$ . Combination of these concentrations (or expressions representing them as  $f(T)$ ) with the determined values of  $D_{Cd}^*$  and  $D_{Te}^*$  or the expressions for these as  $f(p_{Cd}, T)$  as given in Table I leads to the defect diffusion constants as  $f(T)$ . The parameters of these are given in Table II. Parameters for defect diffusion constants in CdS are given for comparison. There is reasonable correspondence between CdTe and CdS for  $D_{V_{Cd}}^-$  as well

as for  $D_{V_{Te}}^-$  and  $D_{V_S^{**}}$ . The latter supports the separation of the native donor  $D_n^{**}$  in  $Cd_i'$  and  $V_{Te}^{**}$  as proposed in (9). The expression for  $D_{Te}^*$  is based on the  $Te_i'$  level being at  $E_v + 0.15$  eV. A higher position of this level (e.g., at  $E_c - 0.58$  eV) would lead to higher  $Te_i^x$  concentrations and lower  $Te_i^x$  mobilities, and the activation energy of  $D_{Te}^*$  would increase to 0.7 eV.

## Summary

Cadmium and Te tracer self-diffusion constants of pure and indium-doped CdTe as  $f(p_{Cd})$  at 700, 800, and 900°C are measured and are analyzed to give contributions by individual point defects. Combination with defect concentrations reported earlier leads to expressions for the diffusion constants of individual defects.

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