

High temperature mobility of CdTe

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The Hall mobility of electrons μ_H is measured in CdTe in the temperature interval 450–1050 °C and defined Cd overpressure in near-intrinsic conditions. The strong decrease of μ_H above 600 °C is reported. The effect is explained within a model of multivalley conduction where both electrons in Γ_{1c} minimum and in L_{1c} minima participate. The theoretical description is based on the solution of the Boltzmann transport equation within the relaxation time approximation including the polar and acoustic phonon intravalley and intervalley scatterings. The Γ_{1c} to L_{1c} separation $\Delta E = 0.29 - 10^{-4}T$ (eV) for the effective mass in the L valley $m_L = 0.35m_0$ is found to best fit the experimental data. Such ΔE is about four times smaller than it is predicted by first-principle calculations. © 2001 American Institute of Physics. [DOI: 10.1063/1.1321774]

The recent progress in high technology brings a renewed interest to the research of the basic properties of CdTe (CT).^{1,2} The purpose of this communication is a study of high temperature near intrinsic mobility evaluated from *in situ* measurements of Hall coefficient R_H and conductivity σ .

In our method the content of Cd in the sample changes due to the sublimation from the free surface. The equilibrium is controlled here by a proper Cd overpressure which is established in the two-zone furnace by a temperature of the Cd source. The advantage of this arrangement is the possibility of measuring properties of CT in the phase P – T diagram both in intrinsic conditions and under Cd or Te overpressure. The measurement of R_H and σ is performed depending on the pressure and temperature of Cd when the equilibrium concentration of electrically active defects is established by diffusion processes. Experimental data show as expected, that R_H and σ depend both on pressure of Cd and temperature, but the μ_H is near intrinsic conditions practically independent of Cd pressure P_{Cd} . It implies that there is no important impurity scattering in this case. Figure 1 shows the phase P – T diagram for CT with a marked region of stability of CT, where our measurements were performed (Cd-rich area of the phase diagram).

The measurement was performed on samples from single crystals prepared by vertical cooling in the temperature gradient. The high temperature measurements were done in a quartz ampoule with a diameter 17 mm located in a furnace between poles of an electromagnet. It was possible to keep the sample temperature with the precision of about 1 °C and to change the gas pressure of one of the components (in our case Cd) in the interval 2×10^{-4} –2 atm. The sample with tungsten or molybdenum spring contacts in the van der Pauw configuration was placed in a quartz holder together with the Pt–PtRh thermocouple.

In this communication we shall concentrate on electrons because the influence of holes is weak and can be included in a simple, standard way. The basic problem at the evaluation

of the drift electron mobility μ at temperatures (500–1000 °C) is the determination of scattering mechanisms, which participate in scattering of current carriers. A number of detailed experimental measurements of mobility were performed at low temperatures (50–300 K), which can be explained well by scattering of electrons on ionized impurities and polar optical phonons.³ The influence of ionized impurities on scattering above 400 K is negligible in pure samples and the dominating scattering on longitudinal optical phonons is expected describing μ in the form

$$\mu = \frac{32\epsilon_0\hbar}{3em} \sqrt{\frac{\pi k_B T}{2m}} \frac{\epsilon_s \epsilon_{opt}}{\epsilon_s - \epsilon_{opt}} \frac{\exp\left(\frac{\hbar\omega_0}{k_B T}\right) - 1}{\omega_0} \times G\left(\frac{\hbar\omega_0}{k_B T}\right) K\left(\frac{E_g}{k_B T}\right), \quad (1)$$

where the effective mass $m = 0.096m_0$, the longitudinal optical phonon energy $\hbar\omega_0 = 21.0$ meV, and the optical and static dielectric constants $\epsilon_{opt} = 7.1$ and $\epsilon_s = 10.3$ are material parameters. The dimensionless function G is calculated according to Ref. 4 and K describes the correction to nonparabolic conduction band within the Kane model.⁵ The mobility is only slightly dependent on ω_0 at high T .

The data of measurements at high temperatures ($T > 500$ °C) published so far^{6,7} however, exhibit substantially stronger decrease of μ_H which reaches above 900 °C less than one half of its theoretical prediction.⁸ Furthermore values from Ref. 7 are $\approx 20\%$ lower than those of Ref. 6. The verification of the experimental data and the explanations of the effect is the main topic of this communication.

Our measurements of Hall coefficient R_H and electric conductivity σ confirm the reliability of values published in Ref. 7 (see Fig. 2).

There are two recommendations found in the literature to explain the fast decrease of μ_H . The first one⁶ expects a strong temperature dependence of material parameters, particularly the static dielectric constant. In agreement with Ref. 8 we do not approve such an explanation. In view of Eq. (1) and the values of the material parameters, ϵ_s would have to

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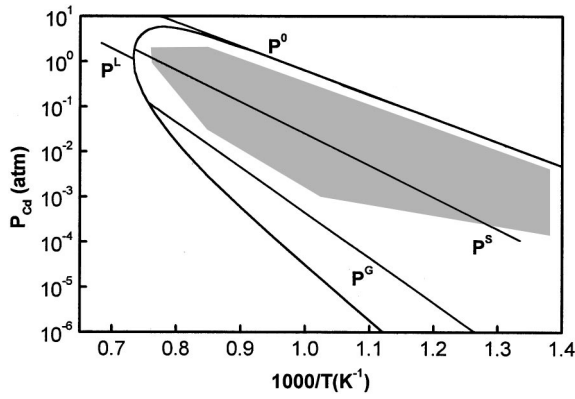


FIG. 1. The P - T phase diagram of CdTe with the marked area (dotted) at which the measurements were performed. P^S , P^G , and P^L plot the solidus, gaseous, and liquidus stoichiometry condition, respectively. P^0 is the Cd partial pressure over pure Cd.

increase twice within the temperature interval 300–1000 °C. Such behavior of ϵ_s is not observed in semiconductors. Also in case of ϵ_{opt} and m their temperature evolution act probably more to the higher than to the lower μ_H .

The second model explanation is based on an assumption of multivalley conduction which comprises both Γ_{1c} minimum and four L_{1c} minima of the Brillouin zone.⁹ The heavier electrons in the L minima reduce μ_H compared to μ_Γ of pure Γ -valley electrons. The similarity to the same effect in GaAs suggests that the Γ_{1c} to L_{1c} separation ΔE may be much less than ~ 1 eV, which is obtained by band structure calculations.^{10,11} Although the idea has been known for a long time, there is no concrete calculation of the high-temperature transport in CT except the numerical modeling of the Gunn effect and hot-electron phenomena.^{12,13} In this communication we attempt to complete the knowledge about CT in this respect, calculating the electron mobility in the Γ_{1c} -valley μ_Γ and L_{1c} -valleys μ_L , as well as the total Hall mobility μ_H at high temperature including the $\Gamma_{1c}+L_{1c}$ intervalley scattering and multivalley conduction.

Our treatment is based on the solution of the Boltzmann transport equation within the relaxation time approximation. The polar optical (PO) phonon and acoustic (AC) phonon as dominant intravalley and intervalley scatterings¹² are used. Due to the intention of studying transport at high T , this approach can be also applied for the optical phonon scattering. To reduce the amount of unknown parameters all valleys are assumed spherical. The corresponding relaxation times τ_{PO} for polar scattering and τ_{AC} for acoustic scattering read

$$\tau_{PO}(E) = \frac{2\pi\epsilon_0}{e^2} \frac{\epsilon_s \epsilon_{opt}}{\partial \Delta k / \partial E} \frac{\exp\left(\frac{\hbar\omega_0}{k_B T}\right) - 1}{\omega_0} G\left(\frac{\hbar\omega_0}{k_B T}\right), \quad (2)$$

$$\tau_{AC}(E) = \frac{\hbar c_l}{\pi E_1^2 k_B T D(E)}, \quad (3)$$

where Δk expresses the single valley dispersion, $c_l = 7 \times 10^{10} \text{ N m}^{-2}$ is the longitudinal elastic constant,¹⁴ and $D = D_\Gamma + 4D_L$ is the total conduction band density of states

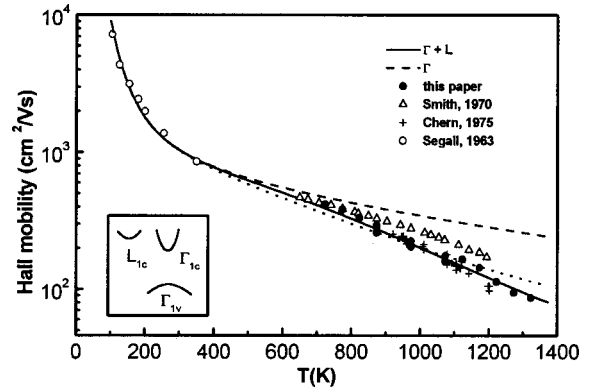


FIG. 2. Experimental and theoretical data of Hall mobilities in CdTe. The low temperature points (\circ) are according to Ref. 3. Our high temperature experiment (\bullet) is shown together with previous measurements (Δ) (Ref. 6) and ($+$) (Ref. 7). Our data confirm the measurements of Ref. 7. The full line draws the best theoretical fit. The dashed line is without effect of the L valley. The dotted line is for temperature independent $\Delta E = 0.19$ eV. The inset plots the scheme of the model band structure.

formed by the single Γ and four L valleys, as well. The intervalley deformation potential is not known in CT, thus we use the intravalley value $E_1 = 4$ eV.¹⁴ This is also the reason why we do not involve other types of scattering in the calculations. Compared to the uncertainty of the material parameters used such an effort would not provide credible improvement of the results. The function G in Eq. (2) expresses the correction to inelastic PO scattering. It also allows τ_{PO} to be used at lower a temperature where $k_B T \sim \hbar \omega_0$. However, such τ_{PO} produces at low T only an approximate Hall factor r_H . The intravalley τ_{PO} can be completed by the intervalley PO scattering terms

$$\tau'_{PO,\Gamma}(E) = \frac{\tau_D}{4D_L(E)}, \quad (4)$$

$$\tau'_{PO,L}(E) = \frac{2\tau_D}{2D_\Gamma(E) + 3D_L(E)}, \quad (5)$$

$$\tau_D = \frac{3\pi\epsilon_0\hbar}{4e^2 k_B T a^2} \frac{\epsilon_s \epsilon_{opt}}{\epsilon_s - \epsilon_{opt}},$$

which yield the relaxation time comparable with τ_{AC} . The k -space intervalley separation is involved through lattice constant $a = 6.48 \text{ \AA}$. The total relaxation time for all valleys is given as

$$\tau^{-1} = \sum_i \tau_i^{-1}, \quad (6)$$

where τ_i label all relevant scatterings [Eqs. (2)–(5)] which yield the Γ and L mobilities. The Hall mobility μ_H is then obtained in the form

$$\mu_H = \frac{r_\Gamma \mu_\Gamma^2 n_\Gamma + r_L \mu_L^2 n_L - r_p \mu_p^2 p}{\mu_\Gamma n_\Gamma + \mu_L n_L + \mu_p p}, \quad (7)$$

where r_Γ , r_L , and r_p are the Hall factors $\langle \tau^2 \rangle / \langle \tau \rangle^2$ and n_Γ , n_L , and p are, respectively, electron and hole concentrations, which are obtained in an obvious way. We found that the fit quality is not influenced significantly by a choice of m_L . We

use $m_L=0.35m_0$ in this communication. This value was successfully used in numerical simulations of the Gunn effect.¹²

The valley separation ΔE is fit to the experimental data. We analyze temperature dependent $\Delta E=\Delta E_0+\alpha T$ which results to the best fit in the form

$$\Delta E=0.29-10^{-4}T(\text{K}) \text{ (eV)}. \quad (8)$$

The results of the calculations together with experimental data are presented in Fig. 2. We see that Eq. (8) describes experimental data quite well. For an estimation of the influence of ΔE to μ_H , the theoretical data for a constant $\Delta E=0.19$ eV are shown by the dotted line in Fig. 2. If we consider possible deviations of material parameters and experimental errors, we estimate the precision of our fit of ΔE_0 to ± 0.05 eV. The T -independent ΔE produces a worse fit with a deviation from the experiment about three times greater than the fit with T -dependent ΔE . Within the estimated experimental precision we cannot, however, confirm $\alpha < 0$ definitely. The $\alpha=0$ produces the fit that expresses the basic character of $\mu_H(T)$ as well. On the other hand, $\alpha > 0$ results in the fit with significant deviations from the experiment.

For comparison, μ_H with the L valley excluded is also plotted in Fig. 2. In Ref. 7, the drift mobility obtained from the Hall mobility using the acoustic-phonon Hall factor $3\pi/8$ was obtained. In view of our Hall mobility presentation we multiplied the data of Ref. 7 by that value to return to μ_H here. Numerical simulation of the Gunn effect¹² was performed with $\Delta E=0.51$ eV and $m_L=0.35m_0$. This ΔE is, however, too high to explain our transport data. For a comparison $\Delta E=0.3$ eV and $m_L=0.22m_0$ are used in GaAs. The value of α in Eq. (8) looks reasonable with respect to the energy gap¹⁵

$$E_G=1.622-3.5\times 10^{-4}T-1.1\times 10^{-7}T^2 \text{ (eV)}. \quad (9)$$

The related ellipsometry measurements and theoretical calculations of α due to thermal expansion and lifetime broadening were reported for GaAs.¹⁶ The results show that α should be negative in GaAs as well, especially due to the lifetime broadening effect.

The effect of the multivalley conduction and the intervalley scattering is demonstrated in Fig. 3. We can distinguish two effects, which reduce μ_H comparing to the single Γ valley transport represented by the line (a). The electrons in the Γ valley at the energy above ΔE scatter strongly into L valleys due to the high density of states there. If these high energy levels are occupied, the mobility μ_Γ is depressed. Such a phenomenon is represented by the line (b). The heavy electrons in the L valley, shown by line (d), are less mobile but their concentration quickly increases at high T . Finally, due to the stronger effect of transport in the L valley to the denominator than to the numerator in Eq. (7), the total Hall mobility drops to its final shape as the line (c).

The involvement of the Hall factors in Eq. (7) influences μ_H significantly. As it is shown in Fig. 3, due to the intervalley scattering the relaxation time is reduced at energy above ΔE which results in the increased r_Γ .

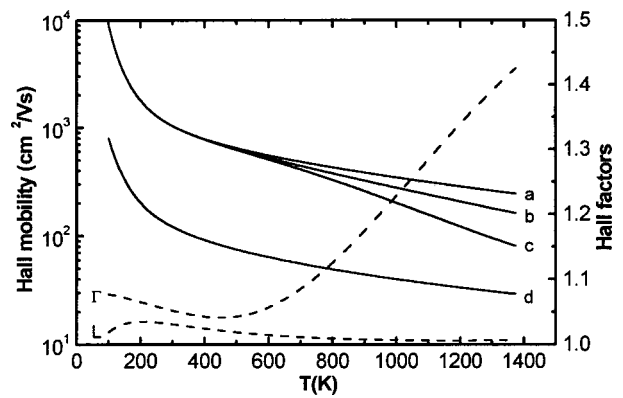


FIG. 3. The Hall mobilities within different types of scattering included (left axis, full) and the conduction band Hall factors (right axis, dash). The mobility μ_Γ without effect of the L valley (line a). The mobility μ_Γ including the intervalley scattering (line b). The total Hall electron mobility (line c). The mobility μ_L (line d). r_Γ (line Γ), r_L (line L).

High temperature *in situ* measurements of mobility in CdTe are reported. The theoretical description of the experimental data is based on the solution of the Boltzmann transport equation within the relaxation time approximation including the polar and acoustic phonon intravalley and intervalley scatterings. The strong decrease of μ_H above 600 °C is explained based on a model of multivalley conduction where both electrons in Γ_{1c} minimum and in L_{1c} minima of the Brillouin zone participate.

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