



Electromigration and Polarization in Schottky Contacts CdTe Based Compounds

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In this work, studies of major transient phenomena, electromigration and polarization, are presented. Electromigration measurements have been carried out at different temperatures on low resistivity p-type CdTe sample with two Au Schottky contacts. Comparative measurements at different temperatures succeeded by etching the anode contact and a thin layer below after each measurement and making a new contact. Temporal conductance of the depletion layer was measured and mobility, acceptor concentrations, diffusion coefficients of the mobile ions and the activation energy of the electromigration process were extracted. Pockels effect technique has been used to study the polarization effect in high resistivity CdZnTe with Au Schottky contacts. Time dependence of Pockels effect measurements was assessed at different temperatures. The analysis of these data revealed that the energy of the deep donor level responsible for the polarization effect in the studied sample is $E_c - 0.8771 \text{ eV}$, with capture cross section $8.71 \times 10^{-13} \text{ cm}^2$.

Keywords: Transient phenomena, CdTe and CZT, Electromigration, Polarization effect

Introduction

During the last decade Cadmium telluride (CdTe) based compounds have been extensively studied due to their wide range of applications [1-8]. In most of these applications, two metals contacts are deposited on CdTe and metal/semiconductor/metal structure (M-S-M) are formed.

In spite of the fact that Schottky type contacts have been used in many applications of CdTe, the temporal change of the physical properties due to the charge dynamics (transient phenomena) often accompanies the material applications. Such phenomena have been considered as of the main reasons responsible for the degradation of the performance of the device and therefore limiting the material applications.

Two major types of transient phenomena in CdTe have been reported:

Polarization phenomena appear typically on a short timescale. This effect has been reported through many years in p-type CdTe detectors [9,10], there are only a few reports on studying the polarization in n-type CZT. In p-type CdTe material, hole de-trapping from deep acceptor level to valence band was reported as a responsible mechanism for polarization phenomena [9-12], The collection properties of the detectors degraded on the short timescale due to this effect [9, 11, 13].

Electromigration phenomena (drift and diffusion of the intrinsic ion under biasing) have been observed on a long time scale [14, 15]. The electromigration of these charged impurities disturbs the stability of

the devices. For example, deterioration of the quality of the HgCdTe infrared detectors has been observed and attributed to the diffusion of the impurities from the CdZnTe substrate [16].

We have carried out Electromigration measurements and developed a new model to explain the phenomenon in CdTe [14]. The electromigrated ions showed no tendency to revert to their initial distribution even after a long time, and therefore, it was impossible to carry out a comparative measurement at different temperatures.

In this work, polarization and electromigration measurements in CdTe and CZT samples with Au contacts are presented. The electromigration measurements were carried out at 323K, 343K, and 363K, where the anode contact has been refreshed after each measurement by etching a thin layer below the anode and a new contact was prepared. Pockels effect measuring technique has been used at several temperatures to study the polarization effect on CdZnTe (CZT) high resistivity sample with two Au contacts.

Theory

Due to the differences in the energy work function of Au and CdTe or CZT, bending of the energy bands took place as Au and CdTe or CZT bulk semiconductor (M-S) are brought into contact and Schottky type junction is formed [7, 17]. Space charge region and electric field are created near the surface of the semiconductor, Fig. (1).

In Au/ low resistivity p-type CdTe (Fig. 1a), the energy bands are bent downwards which may be attributed to the fact that the work function of Au is less than the work function of the p-type semiconductor. According to our model [14], the average electric field, E_d , in the depletion region is assumed to cause electromigration of the charged defects in the depletion region into the semiconductor bulk. This results in a temporal increase in the value of electric field at M-S interface and, therefore, the conductance of the depletion region (G_D) increases with time, with characteristic time is given as

$$\tau_e = \frac{\epsilon \epsilon_0 kT}{q^2 N_A D} \quad (1)$$

Where ϵ is the dielectric permittivity of CdTe (10.3), ϵ_0 is the vacuum permittivity, k is the Boltzmann constant, T is the absolute temperature and D is the diffusion coefficient of donor ions.

The acceptor concentration, N_A , can be determined from the conductivity measurements as follows:

$$\sigma = q N_A \mu_h \quad (2)$$

The hole mobility μ_h at different temperatures in CdTe can be calculated as: [18, 19]

$$\mu_h = 57(e^{252/T(K)} - 1) \text{ (cm}^2\text{V}^{-1}\text{s}^{-1}\text{)} \quad (3)$$

In Au/high resistivity n-type CZT Fig. (1b) the energy bands showed upwards bending due to the fact that the work function of Au is higher than the work function of CZT. According to the model previously developed by the author [7] the application of bias voltage to Au/n-CZT causes sweeps of electrons out from the deep donor level at the depletion volume near the cathode. Therefore, the deep defects positively ionize with a de-trapping time τ , given by the following relation:

$$\tau = \frac{1}{N_C \sigma v} \exp\left(\frac{E_T}{kT}\right) \quad (4)$$

Where $N_C = 2(2\pi m^* kT/h^2)^{3/2}$ and $v = 2(kT/2\pi m^*)^{1/2}$ are the effective density of states at the conduction band edge and thermal velocity of electrons, respectively. E_T is the trap ionization energy relative to the bottom of the conduction band; σ is the electronic capture cross-section.

Material and Methods

Two samples were included in this study: sample S1 was an undoped CdTe bar-shaped with dimensions of 2x3x6.8 mm, and high resistivity CZT sample, S2, with dimensions of 5x5x2.5 mm. The samples were prepared by the Vertical Gradient Freeze method (VGF) [20] in the Technological Laboratory of the Institute of Physics of Charles University in Prague. The sides of the sample were optically polished with final 0.05 mm grit and chemically etched in 1 % Br-methanol solution for 1 min. The contacts were Au and were deposited on the sample by the evaporation method.

The electromigration measurements have been carried out using a four probe method with an additional two contacts, as described in a previous work by the present author [14]. The voltage drop across the depletion region, V_D , was measured, and thus, the temporal variation of the conductance of depletion region, G_D , at different temperatures was recorded as $G_D = I/V_D$, (I is the current passing through the sample). The anode contact and thin layer below was removed by etching after each measurement, and a new anode contact was prepared.

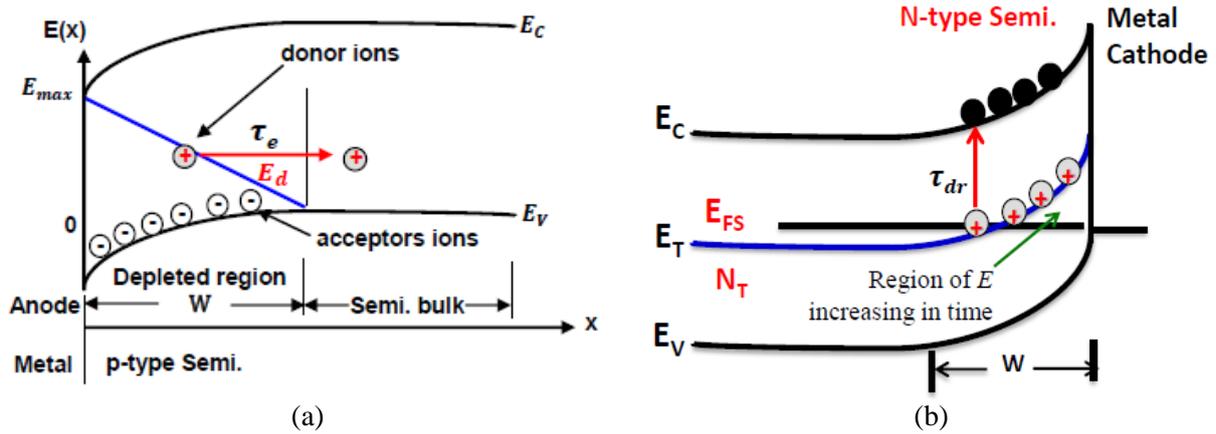


Figure (1): Energy bands diagram showing the bending of the bands at the M-S interface under bias. (a) Au/low resistivity p-type CdTe, (b) Au/high resistivity n-type CZT

Pockels effect technique Fig. (2) was employed to study the polarization effect on CZT high resistivity sample. CZT crystal is exhibiting Pockels effect (linear electro-optic). Using this effect, the distribution of the electric field through the sample can be evaluated using two crossed-polarizers where the light intensity propagating in the direction perpendicular to that of the applied electric field (the polarizers are rotated 45° with respect to the applied electric field) is given by:

$$E(x, y) = \frac{1}{\gamma} \arcsin \sqrt{\frac{I(x, y)}{I_0(x, y)}}, \gamma = \frac{\sqrt{3}\pi n_0^3 r_{41} d}{2\lambda} \quad (5)$$

Where $I(x, y)$ is the distribution of transmitted light intensity; $I_0(x, y)$ is the distribution of the transmitted light intensity with parallel polarizers in case of zero bias; d ($= 5 \text{ mm}$) is the optical path length. λ ($= 980 \text{ nm}$) is the wavelength of the used testing light; $n_0 = 2.8$ is the field free refractive index of CZT (at $\lambda = 980 \text{ nm}$) and r_{41} ($= 6.5 \times 10^{-12} \text{ m/V}$) is the linear electro-optic coefficient.

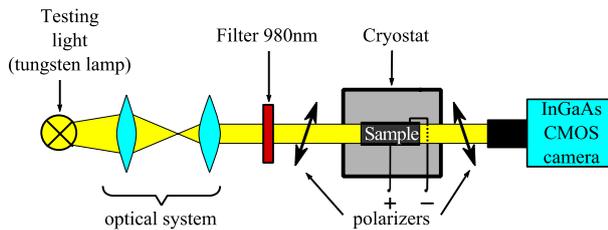


Fig. (2): Pockels effect setup employed to study the polarization effect on CZT high resistivity sample. Collimated testing light cut by narrow band filter at 980 nm passes through the biased CZT sample situated between two crossed polarizers is sensed by NIR InGaAs CCD camera nm passes through the biased CZT sample situated between two crossed polarizers is sensed by NIR InGaAs CCD camera

Results and Discussion

Electromigration measurements

The electromigration measurements have been carried out on the low resistivity sample, S1. The temporal variation of the conductance of depletion region, G_D ($= \frac{I}{V_D}$) at 363K, 323K and 343K were measured by monitoring the voltage drop across the depletion region, V_D . After each measurement, the anode contact and few micrometers thin layer below were removed and a new contact was prepared to have a similar distribution of ions before each measurement. Fig 3 shows the data of these measurements together with the exponential fit, (solid lines), the characteristic time at different temperatures is shown in table 1.

The acceptor density N_A at the measured T was determined from the conductivity σ using eq. (3) and the values of the diffusion coefficient of donor ions were extracted using eq. (2) and are presented in table 1. These values are in agreement with the values of diffusion coefficients of ions: Ag, Na, Cu and K in CdTe with a similar carrier concentration using transient ion drift (TID) method [21]. The diffusion coefficient extracted here, in this manuscript, could be attributed to one of these elements.

The activation energy of the electromigration process, E_a , can be determined using the Arrhenius equation $D(T) = D_0 e^{-E_a/kT}$ (D_0 is the pre-exponential factor). The insert of Fig. (3) shows the Arrhenius plot with excellent straight line fit. The activation energy was found to be 0.36 eV.

Table (1): The values of characteristic time (τ), conductivity (σ), acceptor concentration (N_A) and the diffusion coefficient (D) at different temperatures (T)

T (K)	τ ($\times 10^3$ s)	σ ($\times 10^{-3}$ S/cm)	N_A ($\times 10^{14}$ cm $^{-3}$)	D ($\times 10^{-13}$ cm 2 s $^{-1}$)
323	3.133	2.15	2.00	2.54
343	2.604	1.05	1.35	4.80
363	1.395	0.83	1.25	10.2

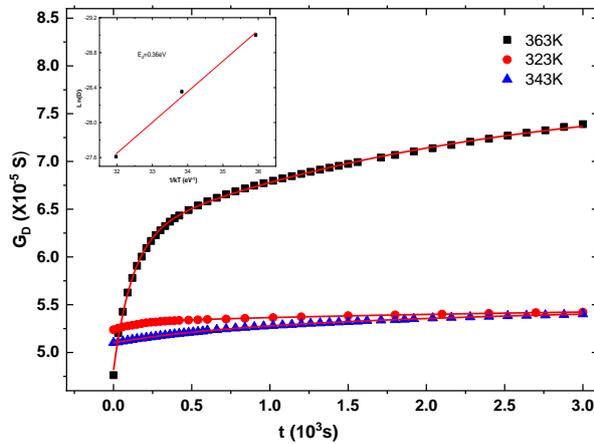


Figure (3): The measured conductances of the depletion region at different temperatures. solid lines represent the exponential fit of the Measurements. The insert is the Arrhenius plot of the diffusion coefficient

Polarization measurements

The distribution and the stability of the electric field in the CZT sample (S2) are studied by employing the Pockels effect technique and using equation (5). The profiles of the internal electric field during 80 minutes in the sample at 300K and bias 250 V are presented in Fig. (4). One can note that the E- field is confined below the cathode (reverse biased contact), which corresponds to the presence of positive space charge in the sample volume. It is also noted that the E- field moves with time towards the cathode side and is confined in a region of about 10% of the sample thickness after about 30 minutes from applying the bias.

The value of the E-field at the Au/CZT cathode interface (E_0) increases with time as a result of increasing the positive space charge with time near the cathode. The de-trapping of electrons from deep donor level is reported [7] as responsible for this effect. The de-trapping time of this process is given by eq. (4).

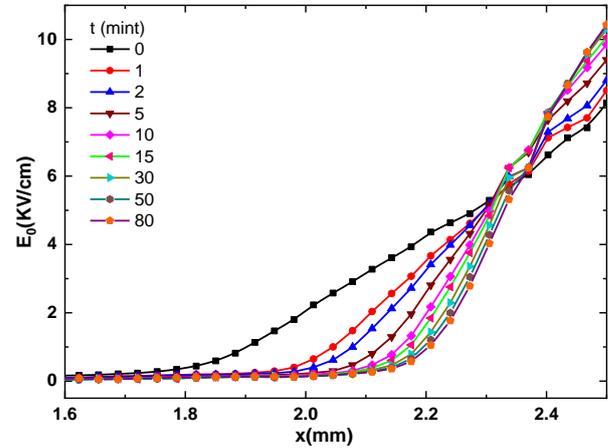


Fig. (4): Temporal distribution of the electric field in CZT sample acquired by Pockels measurements at 250V bias and 300K

To determine the energy and capture cross section of the deep donor level responsible for polarization, temporal Pockels effect measurements were carried out at different temperatures. Fig. (5) shows the time dependence of the values of E_0 (at Au/CZT interface) at different temperatures. The electronic de-trapping time at different temperatures Table (1) was extracted from the exponential fits of the data in Fig 5. From the Arrhenius plot of $\ln(1/\tau T^2)$ versus $1/kT$ – (insert of Fig. 5), the activation energy of the deep level responsible for the polarization was found to be $E_T=0.877$ eV.

From eq. (4), the intercept of the resulting straight line of Arrhenius plot is at $\ln(\sigma N_C T^2)$. The intercept of the straight line in the insert of Fig. 7. is at 16.92, thus, the capture cross-section of the trap was found to be $\sigma = 8.7 \times 10^{-13}$ cm 2

In p-type CdTe sample, a hole trap of energy $E_V+0.62$ was responsible for a polarization mechanism [22]. In this work (n-type CZT sample) the polarization was attributed to the deep level of energy $E_C-0.877$ eV. It is noticed that the sum of both energies is about 1.50eV, which equals the energy bandgap of CZT (at room temperature). It is reasonable to deduce that the origin of this deep trap may be the same in both n-type and p-type of samples. In case of CdTe: Cl samples with In

contact, it can emit holes (the bands are bent downwards) however, in the opposite case, our case, CZT with Au contacts it emits electrons (when the bands are bent upwards).

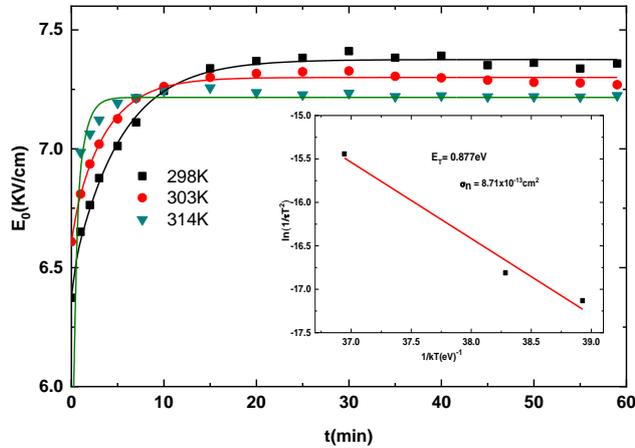


Figure (5): Temporal of the electric field at the Au/CZT cathode interface at 200V and at different temperatures- Insert plot shows the Arrhenius plot of the values of the electronic de-trapping time extracted from the data of Fig. (5)

Table (2): Electronic de-trapping time (τ) at different T

T (K)	time τ (s)
298	310
303	217
314	51

Conclusions

The comprehensive study of electromigration in p-type CdTe with two Au contacts is presented. Temporal measurements of the conductivity of the depletion layer were performed at different temperatures. Diffusion coefficients of the ion were extracted at different temperatures, and the activation energy of the electromigration process was found to be 0.36eV. The polarization phenomenon in n-type CdZnTe with two Au contacts was investigated using the Pockels effect technique. Temperature-dependence of the temporal Pockels effect measurements were carried out to study dynamics of the internal electric field profiles across the studied structure. We further found parameters of the deep electronic trap such as energy E_c -0.877 eV and electronic capture cross section $8.7 \times 10^{-13} \text{ cm}^2$. We showed that this deep level is responsible for the polarization of

semiconductor device. The deep level parameters, electromigration, and polarization dynamics presented in this research are crucial for the development of the radiation detector technology.

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