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Abstract. In order to get information about the deep levels of a semiconductor from
photoinduced current transient spectroscopy (PICTS), the thermal relaxation times must
be calculated from the time dependence of the photoinduced current. If the deep levels
have a bandwidth their contribution to the photoinduced current must be described by
a relaxation time spectrum. In this case a regularization method as implemented, for
example, in the program FTIKREG should be used for the calculation. The advantages
of the regularization method in comparison with the customary two-gate technique are
demonstrated by the analysis of simulated and real experimental data. The experimental
data have been obtained from a high-resistivity CdTe:Br crystal.

1. Introduction

Photoinduced current transient spectroscopy (PICTS or PITS) [1] has been used for
several years to investigate deep levels in high-resistivity semiconductors. For that
purpose the time dependence of the photoinduced current I given by [2,3]

$$I(t) = I_0 + \sum_{i=1}^{n} h_i \frac{e^{-t/\tau_i}}{\tau_i} \tag{1}$$

is measured at several temperatures. In (1) n is the number of distinct deep levels, I_0
denotes the dark current and the coefficients h_i specify the contribution of each level
to the photoinduced current. The temperature dependence of the thermal relaxation
times

$$\tau_i^{-1} \sim \sigma_i T^2 e^{-\Delta E_i/k_B T} \tag{2}$$

(k_B denotes the Boltzmann constant) provides the information on the deep levels,
namely the activation energy ΔE_i and the cross section σ_i. The purpose is, therefore,
to determine the thermal relaxation times τ_i from the photoinduced transients at
various temperatures.

Essentially the same problem arises in the analysis of deep-level transient spec-
troscopy data (DLTS) [4]. In this context various methods (two-gate [4] and four-gate
[5] technique, Fourier methods [6], MEDLTS [7], direct fitting [8]) have been proposed

for the analysis of the transients. The large variety of methods shows however, that no satisfactory method has been proven most effective until now.

In this paper we use a regularization method for the determination of the thermal relaxation times similar to a method recently used for the evaluation of DLTS data [9, 10]. This method reveals levels that cannot be resolved by the usual methods. In addition, with this method the number of active levels at a given temperature can be determined with one isothermal measurement. The advantages of the regularization method in comparison with the customary two-gate technique are demonstrated by the analysis of simulated and real experimental data. The experimental data have been obtained from a high-resistivity CdTe:Br crystal. High-resistivity CdTe has a wide range of applications, as e.g. room temperature gamma-ray detectors [11] and high efficiency solar cells [12].

In the following section the evaluation of the photoinduced transients with the regularization method is described. In section 3 the method is tested using simulated data. Section 4 includes experimental details concerning the data that are used in section 5 for the demonstration of the advantages of the regularization method.

2. Method of data analysis

The starting point for the analysis of PICTS data by a regularization method is the possibility that the deep levels may have a bandwidth. In this case the contribution of the deep levels to the photoinduced current I must be described by a relaxation time spectrum:

$$I(t) = I_0 + \int_{-\infty}^{\infty} h(\ln \tau) e^{-t/\tau} \, d(\ln \tau). \tag{3}$$

For each deep level the relaxation time spectrum $h(\ln \tau)$ is expected to show a peak. The size of the peak characterizes the contribution of the corresponding deep level to the photoinduced current I, the peak width depends on the bandwidth, and the activation energy ΔE_i and the cross section σ_i can be calculated from the temperature dependence of this peak.

In practice the spectrum $h(\ln \tau)$ must be calculated from noisy data for the photoinduced current I. As (3) is up to the constant I_0 a Fredholm integral equation of the first kind, this problem is known to be ill-posed (see [15] for a definition of ill-posed problems) and specific solution methods such as Tikhonov regularization [16] must be used to solve it.

With Tikhonov regularization an estimate for the spectrum $h(\ln \tau)$ and the constant I_0 is obtained from noisy experimental data $I_1^\sigma, \ldots, I_n^\sigma$ for $I(t_1), \ldots, I(t_n)$ with errors $\sigma_1, \ldots, \sigma_n$ (for the experimental data an absolute error $\sigma_i = \sigma$ was assumed) by minimizing

$$V(\lambda) = \sum_{i=1}^{n} \frac{1}{\sigma_i^2} \left(I_i^\sigma - \left(I_0 + \int_{-\infty}^{\infty} e^{-t/\tau} h(\ln \tau) \, d(\ln \tau) \right) \right)^2 + \lambda \, \| h \|^2 . \tag{4}$$

In this equation the so-called regularization parameter λ has been introduced. With an appropriate value for this parameter, the first term on the right-hand side of (4) forces the result to be compatible with the data. The second term leads to a smooth estimate for the spectrum $h(\ln \tau)$.

This method has been used successfully, e.g. for the analysis of quasi-elastic light scattering data [17] and rheological data [18]. In either case a relaxation time spectrum related to the experimental data by an equation analogous to (3) must be determined. For the calculations programs such as CONTIN [19, 20] or FTIKREG [21] are available.

The calculations in the following sections have been performed with the program FTIKREG which has been developed by one of the authors. Given noisy experimental data and the corresponding data errors, the program FTIKREG computes the approximate solution of equations analogous to (3) defined by Tikhonov regularization. In addition FTIKREG offers several features, such as the ability to estimate the optimal value of the regularization parameter λ with the SC-method [22, 23]. This feature is very important, because it depends mainly on this parameter, whether the result obtained by a regularization method is good or not. Furthermore, the ability to calculate a positive solution of (3) was used.

3. Testing the method with simulated data

In order to check the accuracy and the resolution of the regularization method, data for the transients containing contributions of three different levels were generated. With the level parameters summarized in table 1 the photoinduced current I was calculated for six temperatures (104 K, 106 K, 108 K, 110 K, 112 K, 114 K) according to

$$I(t) = \sum_{i=1}^{3} h_i \frac{e^{-t/\tau_i}}{\tau_i} \tag{5}$$

$$\tau_i^{-1} = F_i T^2 e^{-\Delta E_i / k_B T}. \tag{6}$$

Table 1. Parameters used to generate the simulated data.

	ΔE_i (eV)	F_i (K^{-2} s^{-1})	h_i
Level 1	0.16	8.7 × 10^5	5.0
Level 2	0.17	8.7 × 10^5	10.0
Level 3	0.18	8.7 × 10^5	2.0

The simulated data were obtained by evaluating the current I at 1024 points with $0.0002 \text{ s} \leqslant t \leqslant 0.2048 \text{ s}$ and $\Delta t = 0.0002 \text{ s}$. The experimental error was simulated by adding a Gaussian random number corresponding to an absolute error of 1.0. A typical data set for the photoinduced current I and the corresponding relaxation time spectrum $h(\ln \tau)$ calculated with the program FTIKREG are shown in figure 1.

The relaxation time spectrum (figure 1(b)) shows three narrow peaks. The size of each peak provides information about the contribution of the corresponding deep level to the photoinduced current I. The position of each peak characterizes the thermal relaxation time τ_i. An estimate τ_i^σ of the thermal relaxation time τ_i was calculated according to

$$\tau_i^\sigma = \int_{\text{peak}} \tau h(\ln \tau) \, \mathrm{d}(\ln \tau) \bigg/ \int_{\text{peak}} h(\ln \tau) \, \mathrm{d}(\ln \tau). \tag{7}$$

Table 2. Estimates τ_i^σ of the relaxation times τ_i obtained from the relaxation time spectra. The last column includes the corresponding error.

$\tau_i(T)$ (s)	$\tau_i^\sigma(T)$ (s)	error (s)
$T = 104$ K		
5.93×10^{-3}	5.94×10^{-3}	7.8×10^{-5}
1.81×10^{-2}	1.80×10^{-2}	1.8×10^{-4}
5.51×10^{-2}	5.63×10^{-2}	1.1×10^{-3}
$T = 106$ K		
4.08×10^{-3}	4.12×10^{-3}	4.3×10^{-5}
1.22×10^{-2}	1.23×10^{-2}	9.9×10^{-5}
3.63×10^{-2}	3.73×10^{-2}	4.6×10^{-4}
$T = 108$ K		
2.84×10^{-3}	2.84×10^{-3}	2.7×10^{-5}
8.31×10^{-3}	8.35×10^{-3}	5.7×10^{-5}
2.43×10^{-2}	2.49×10^{-2}	2.3×10^{-4}
$T = 110$ K		
2.00×10^{-3}	2.00×10^{-3}	2.2×10^{-5}
5.75×10^{-3}	5.76×10^{-3}	4.0×10^{-5}
1.65×10^{-2}	1.69×10^{-2}	1.7×10^{-4}
$T = 112$ K		
1.43×10^{-3}	1.45×10^{-3}	1.3×10^{-5}
4.03×10^{-3}	4.06×10^{-3}	2.4×10^{-5}
1.13×10^{-2}	1.16×10^{-2}	8.6×10^{-5}
$T = 114$ K		
1.03×10^{-3}	1.03×10^{-3}	7.5×10^{-6}
2.85×10^{-3}	2.86×10^{-3}	1.4×10^{-5}
7.89×10^{-3}	8.01×10^{-3}	3.6×10^{-5}

Figure 2 shows an Arrhenius plot of the estimates τ_i^σ obtained from the relaxation time spectra $h(\ln \tau)$. In addition these estimates are listed in table 2. This table includes an estimate of the corresponding error. These values have been used to determine the parameters of the deep levels by a non-linear least-squares method [24]. The result shown in table 3 agrees well with the values used to simulate the data (table 1).

Table 3. Parameters of the deep levels calculated from the estimates τ_i^σ of the relaxation times τ_i in table 2.

	ΔE_i (eV)	F_i (K^{-2} s^{-1})
Level 1	0.1597 ± 0.0013	$(8.6 \pm 1.2) \times 10^5$
Level 2	0.1698 ± 0.0009	$(8.6 \pm 0.8) \times 10^5$
Level 3	0.1808 ± 0.0012	$(9.5 \pm 1.1) \times 10^5$

In order to emphasize the advantages of the regularization method the data have also been evaluated with the conventional two-gate technique [4]. The corresponding PICTS spectra (an example is shown in figure 3) indicate only one deep level with $\Delta E = (0.175 \pm 0.002)$ eV and $F = (1.4 \pm 0.3) \times 10^6$ K^{-2} s^{-1}. These parameters characterize level 2 (table 1). Level 1 as well as level 3 cannot be recovered by the two-gate technique.
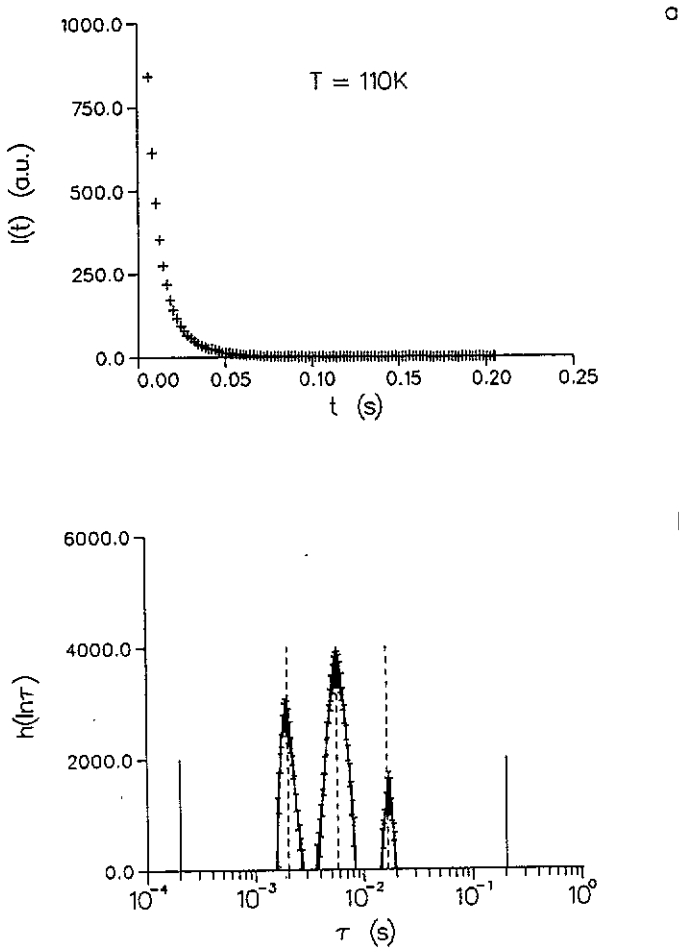
Figure 1. Typical data set for the photoinduced current $I(t)$ (a) and corresponding relaxation time spectrum $h(\ln \tau)$ calculated with FTIKREG (b).
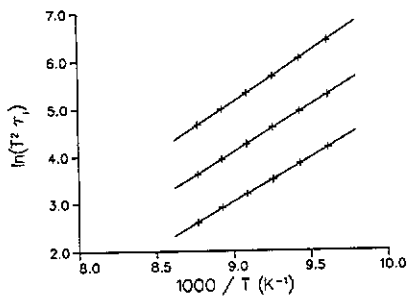

Figure 2. Arrhenius plot of the estimates τ_i^{σ} of the relaxation times τ_i obtained from the simulated data.

4. Experimental details

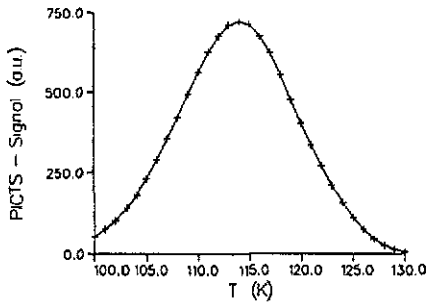The experimental data have been obtained from a Bridgman-grown CdTe crystal

Figure 3. Typical PICTS spectrum ($t_2/t_1 = 2$) for the simulated data. Only one of the three levels can be recovered with the two-gate technique.

doped with Br_2 [13]. The crystal was n-type with a dopant concentration of 2×10^{18} cm^{-3}. As this dopant compensates electrically active native defects (see [25] for a detailed description of the compensating mechanism) the crystal had a high specific resistivity of 4×10^9 Ω cm. For the measurement the crystal was cut into wafers of thickness 1 mm, mechanically polished down to 1 μm and etched for 30 s with a 10 vol% bromine–ethanol solution. Then, Au was evaporated on one side and In on the other in order to obtain good electric contacts.

For the PICTS analysis an experimental set-up as described in [14] was used: the sample was placed in a nitrogen cryostat which allows temperature control in the range of 70 to 350 K within 0.1 K. It was excited by a laser diode with a wavelength of 830 nm (below-bandgap excitation) and a computer-controlled pulse width between 60 and 200 ms. Applying a variable DC voltage to the sample the photoinduced current was measured with a fast current amplifier connected to a fast AD/DA converter in a PC. In this way the photoinduced current was recorded at N equally spaced points with a difference Δt. Typical values for N and Δt are given by $N = 1024$ and $\Delta t = 1 \times 10^{-4}$ s.
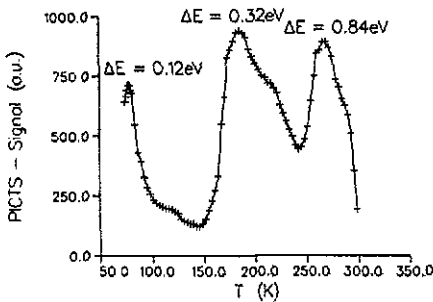

Figure 4. PICTS spectrum ($t_2/t_1 = 2$) calculated from the experimental data for the CdTe:Br crystal.

5. Experimental results

Figure 4 shows a PICTS spectrum calculated with the conventional two-gate technique from the experimental data. This spectrum shows three resolvable peaks in the
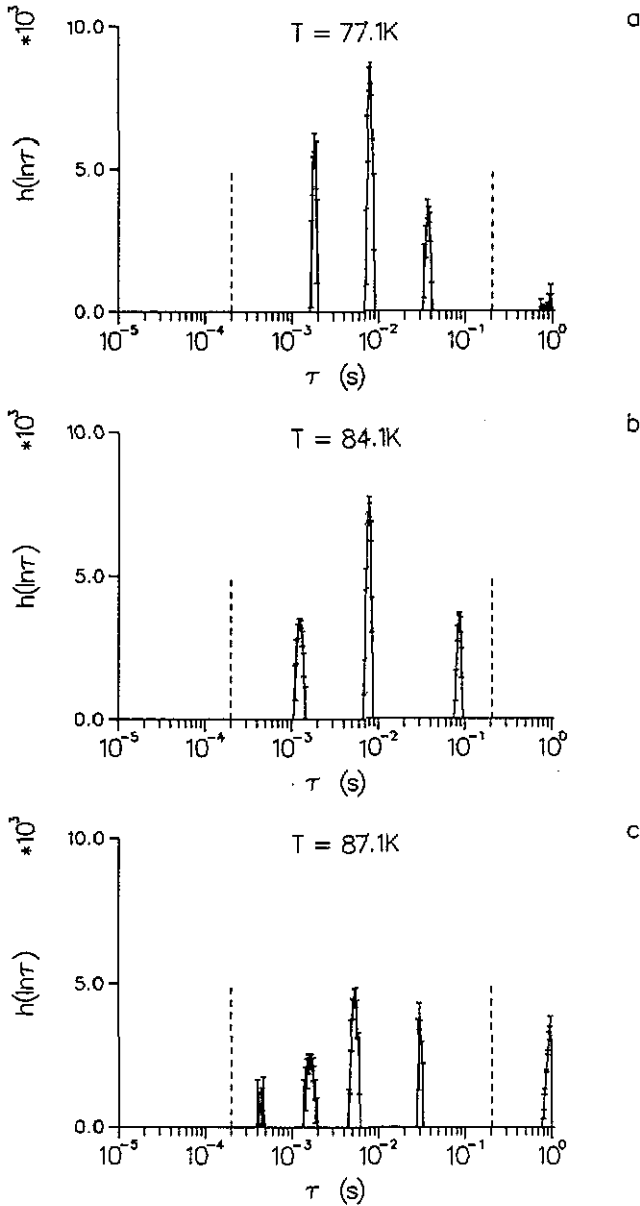
Figure 5. Typical relaxation time spectra $h(\ln \tau)$ calculated from the experimental data for the CdTe:Br crystal.

temperature range of 74–300 K. These peaks correspond to deep levels with an activation energy of $\Delta E = 0.12$ eV, $\Delta E = 0.32$ eV and $\Delta E = 0.84$ eV.

Detailed results on CdTe:Br are not available in the literature. The deep levels can therefore only be interpreted in reference to results obtained for CdTe:Cl. Levels in the 0.1–0.2 eV range can therefore be attributed to compensation defects [26]. A definite identification of the level with $\Delta E = 0.32$ eV is not yet available. Possible origins may be a Te vacancy or residual chemical impurities like Cu, Ag and Au. The

last level is caused by the V_{Cd}^{2-} defect [27].

In order to show the capabilities of the regularization method, a detailed analysis of the level with $\Delta E = 0.12$ eV was performed. For that purpose the experimental data obtained at temperatures between 77 and 110 K have been evaluated as described in section 2. Some typical relaxation time spectra, $h(\ln \tau)$, are shown in figure 5. From these spectra estimates τ_i^σ for the relaxation times τ_i and the corresponding errors were calculated. Figure 6 shows an Arrhenius plot of the result. Altogether five different deep levels could be recovered. The parameters of these levels calculated from the relaxation times τ_i^σ are listed in table 4.

Table 4. Parameters of the deep levels of the CdTe:Br crystal.

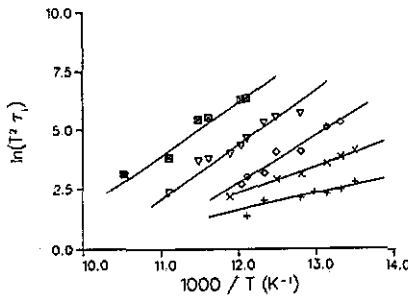|	ΔE_i (eV)	σ_i (cm^2)
Level 1	0.0604 ± 0.0089	$(2.6 \pm 3.3) \times 10^{-18}$
Level 2	0.0989 ± 0.0014	$(2.8 \pm 0.5) \times 10^{-16}$
Level 3	0.1731 ± 0.0005	$(5.5 \pm 0.4) \times 10^{-12}$
Level 4	0.2003 ± 0.0008	$(4.8 \pm 0.6) \times 10^{-13}$
Level 5	0.1957 ± 0.0009	$(4.3 \pm 0.5) \times 10^{-13}$

Figure 6. Arrhenius plot of the estimates τ_i^σ of the relaxation times τ_i for the CdTe:Br crystal.

According to the literature [11] level 1 can be correlated to the $V_{Cd}^{2-}2Br_{Te}^{+}$-complex lying 0.06 eV below the conduction band. The other levels are part of the so-called 0.15 eV acceptor band [28]. The levels in this band are caused by compensating defects and lead to a high resistivity of the material [30]. Results for chlorine-compensated materials [26] lead to the conclusion that these defects in CdTe:Br have two main constituents, namely cadmium vacancies and bromine. Our results for the CdTe:Br crystal indicate however that the defect structure of the 0.15 eV band is more complex. The actual structure may vary from a $Br^+ V_{Cd}^{2-}$ to a more complex $(Br_n^+ V_{Cd}^{p-} X^{q\pm})^{k-}$ bonding where X is an impurity and n, p, q and k are multiples of elements and the charge state, respectively. Since PICTS is only a method for detecting deep levels a closer investigation of the chemical structure of the observed defects has to be done with other methods e.g. ESR.

6. Conclusions

For the analysis of PICTS data, we have proposed calculating a relaxation time spec-

trum from the data for the photoinduced current. This calculation can be done with a regularization method as implemented, e.g., in the program FTIKREG. From the temperature dependence of the peaks in this spectrum the parameters of the deep levels can be determined. The method has been tested with simulated data. In addition the method has been used to analyse data for a CdTe:Br crystal. The results show that the regularization method is much more sensitive for levels with a relatively low concentration than the conventional two-gate technique.

For different levels with similar cross section and activation energy the two-gate technique is only able to detect the level with the highest concentration. The results obtained in this way indicate, therefore, that different samples of the same material have different deep levels. In contrast to this, the results calculated with the regularization method may indicate that different samples of the same material have the same deep levels with varying concentration. The investigation of this question may be the subject of further work.

Acknowledgment

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