

## Numerical Approach to the Problem of Digital DLTS Measurements Signal analysis

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### Abstract:

This paper presents a novel approach in the investigation of the parameters of deep energy levels in digital DLTS (Deep Level Transient Spectroscopy) measurements. A DLTS spectra fitting algorithm and by this the calculation of the activation energy capture cross section and the trap concentration of deep energy levels is proposed. As a final result the match between fitted and evaluated parameters are presented. The fitted curves are used as representatives for a peak in the DLTS spectra. The measured DLTS signals were used for the results comparison of the numerical fitting approach and the standard DLTS direct evaluation method.

### INTRODUCTION

The DLTS technique originated by Lang [1] in 1974 is a method for the material defect characterization. A structure with a barrier, usually Schottky diode is measured. A short voltage pulse is applied to the structure which fills-up the deep energy level states (so called defects) in the material structure of the sample. Immediately after that a capacitance transient is being measured which corresponds to the capture and emission processes in the material activated by an applied voltage pulse. This is repeated in desired range of temperatures, so the result is a set of the capacitance transients measured at each temperature value. The measured capacitance transients represent decays of the capacitance of the measured structure, corresponding to the charge changes and the capture and emission processes in the material defects. The rate window is applied to all measured transients and resulting capacitance difference is plotted as DLTS spectra. The spectra usually consist of peaks that represent the deep energy levels. By further analysis the parameters of the deep energy levels are obtained out of the corresponding Arrhenius plot.

The deep energy level parameters calculation in the original DLTS is carried out by simple analog devices. Conventional techniques of DLTS like the double boxcar average [1], the lock-in amplifier response [2, 3], or exponential correlation [2, 4] use analog instruments such as Fourier analyzers, integrators, and correlators. There are no transient, just two values of the capacitance are measured and processed, so the output is either the difference between two points or a convolution of the capacitance signal. In all these methods, the primary signal, the capacitance transient, is lost during the signal processing. Each temperature scan results in

one DLTS spectra and therefore only one data point on the Arrhenius plot for the deep energy level, and hence multiple temperature scans are required in order to obtain enough points on the Arrhenius plot to accurately estimate the characteristics of the deep energy level [5]. In the time when the original technique was introduced its precision was satisfying and its simplicity was a big advantage. Over the years the material science and semiconductor industry developed rapidly. Nowadays, the precision of the original DLTS technique is sometimes not enough. Due to the availability of the fast and powerful computing options the simplicity of the algorithm is not so important any more. Many variations of the original method were introduced to achieve better energy resolution of the DLTS method. Some of them use Fourier or Laplace analysis [6] in defect investigation, which pushes further the ability of the DLTS method to recognize multiple deep energy levels in the measured structure and so to calculate their parameters (activation energy, capture cross-section and trap concentration).

The problem of the composite signals in the digital DLTS systems is well known and dealt with in several approaches. When dealing with the new progressive materials or generally semiconductor materials with high density of defect states in the material lattice, often question arises how to distinguish individual signals coming from each deep energy level emission. The problem is that the output signal is a composite of all the signals coming from the emissions of all deep energy levels. It is not simple to separate such composite signals and calculate accurate trap parameters, sometimes even impossible to do so, especially when the deep energy levels are very close to each other.

## NUMERICAL APPROACH

### General idea

A numerical approach that tries to deal with the problem of composite signal separation was proposed and briefly discussed in one of our previous papers [7]. A presented approach in this paper represents the next and improved version of this evaluation algorithm, especially the calculation of the defect parameters based on a precisely fitted DLTS curve, depicting the exact character of the measured data. It looks into the problem from a different perspective using only numerical characterization of the peaks present in the measured DLTS spectra. The mentioned approach [7] is a suitable tool for the separation of composite DLTS signals but needs to be enhanced also with a numerical calculation of the basic parameters of deep energy levels, namely the activation energy the capture cross section and the trap concentration.

Typical measured DLTS spectra consists of one or more peaks. In case of one peak present in the spectra, naturally, there is no composite signal and separation is not needed. Although if the peak is very wide and its shape suggests that it actually consists of two individual peaks the separation is needed. The same applies when a DLTS spectrum consists of more than two peaks, either it's clear to distinguish them or not. A typical DLTS peak corresponding to one deep energy level in the DLTS spectra has a symmetric "bell curve" shape, which was previously defined as a Gaussian (or normal) distribution function [7]. In our new approach presented in this paper it is defined as a function based on the standard physical model of emission and capture processes in semiconductors [8]. This function is defined according to the mentioned trap parameters and has the following form:

$$S(\Delta E_a, \sigma_n, N_T, T) = \frac{2}{T_w} \frac{C_R N_T}{2N_S} \int \exp\left(-\frac{t}{\tau_e(\sigma_n, \Delta E_a)}\right) W_{SL} dt \quad (1)$$

where  $\Delta E_a$  is the activation energy,  $\sigma_n$  is the capture cross section,  $N_T$  is the trap concentration,  $T$  is the temperature,  $W_{SL}$  is the correlation function (weighting function),  $C_R$  is the reverse capacitance at 0 V and  $N_S$  is the doping concentration in the substrate [8]. In the presented model the "Square Lockin" correlation function shown in the Fig.1 was used, and defined according to the DLTS measurement system's user manual and literature [9].

By changing the  $S$  function parameters one can obtain any desirable shape of the DLTS spectrum, similar to the measured signals. Thus we can define defect parameters (corresponding to a deep energy level) in the DLTS spectra by a set of specific  $S$  function parameters.

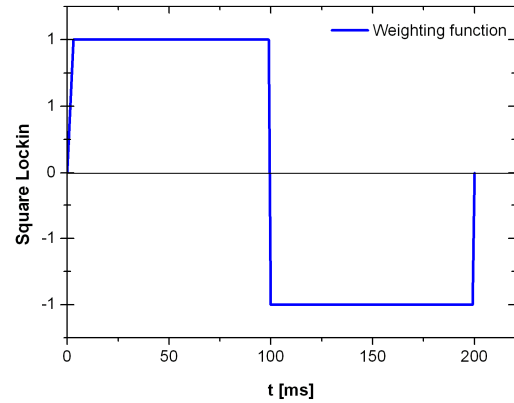


Fig.1 Square Lockin weighting function

### Calculation and fitting

The presented numerical fitting algorithm is based on a so called "Temperature fit" process, which includes a reverse calculation of the DLTS spectra by the mentioned function  $S$  [8] based on the deep energy level parameters. This simulation process of the DLTS spectrum is a suitable tool for the verification of the evaluated trap parameters obtained by other methods and also as an alternative for the calculation of these values. In accordance to these facts an automatic (calculation tool) and also a manual (verification tool) algorithm had been tested.

These two modules of the presented algorithm were designed based on the solution of the mentioned  $S(\Delta E_a, \sigma_n, N_T, T)$  function, which is basically a loop cycle with equations determining the emission rate by Eq. (3), thus the emission time constant of charge carriers Eq. (2), for a specific set of function parameters and material constants Eq. (4). Here  $v_{th,n}$  is the thermal velocity and  $N_C$  is the density of states for the correct values of effective masses.

$$\tau_e = \left( \sigma_n v_{th,n} N_C \exp\left(-\frac{E_C - E_T}{kT}\right) \right)^{-1} \quad (2)$$

$$e_n = 1/\tau_e \quad (3)$$

$$v_{th,n} = \sqrt{\frac{3kT}{m_n^*}} \quad N_C = 2M \left( \frac{2\pi m_n^* kT}{h^2} \right)^{\frac{3}{2}} \quad (4)$$

The manual module of the program requires the user to manually edit the simulation input data, specifically the trap parameters obtained from e.g. DLTS measurement unit's software evaluation. The resulted function compared to the measured DLTS spectrum ensures the verification of the evaluated data. If set, these manually added input values are also used at the automatic module of the proposed

algorithm where various combinations of the trap parameters (activation energy, capture cross section, trap concentration) are generated to determine a more precise curve. If these data are not set the automatic algorithm tries to calculate the curve starting the loop function with a defined set of parameters.

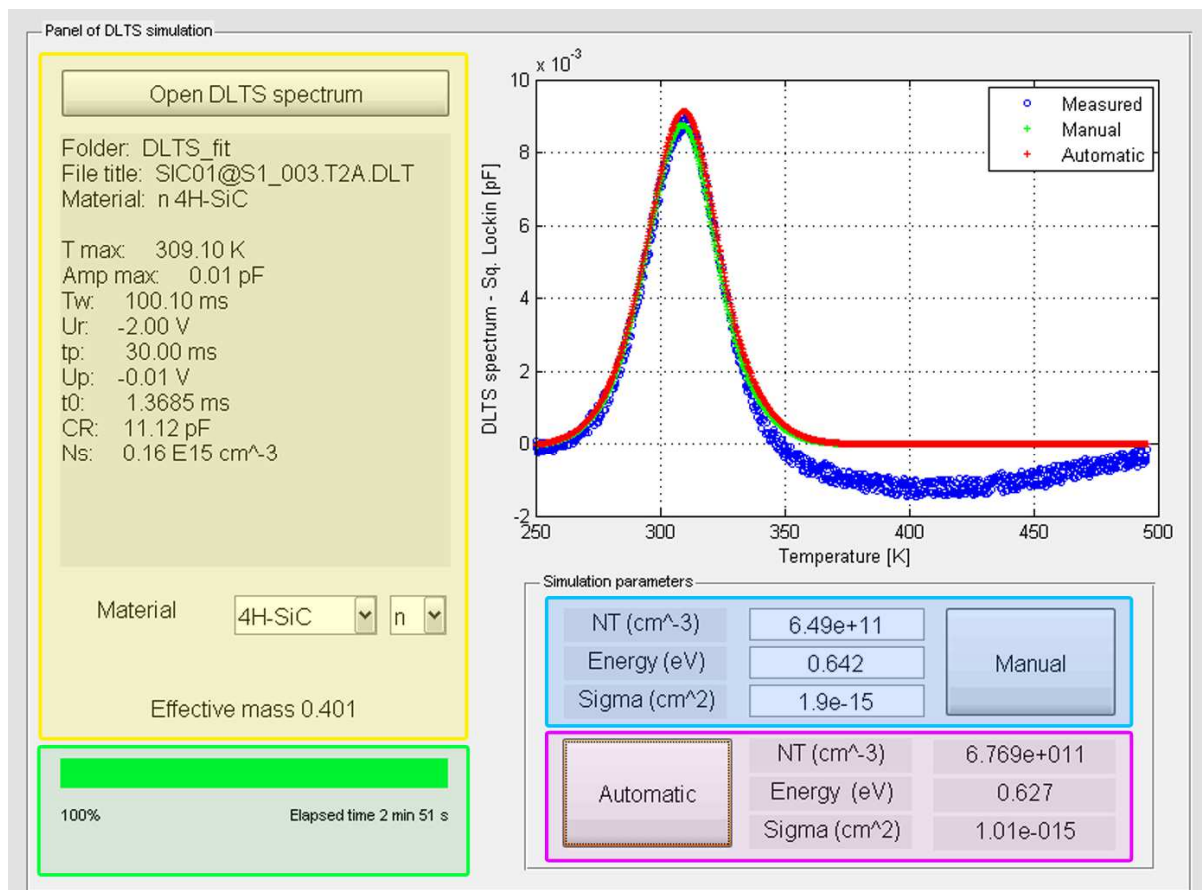
The precision between the generated and measured DLTS curves is ensured by the comparison of its three variables, the position of the peak maximum, the amplitude and the width at half of the peak maximum. If the difference in the compared spectra is within the tolerance parameter the fitting loop ends, otherwise it repeated until the conditions are fulfilled. Of course, there is a possibility that the fitting loop will end without getting into the tolerance that is without the result. In this case the input parameters need to be changed and fitting process repeated.

The final result of the fitting algorithm is the calculated signal (DLTS spectra) that was the most

accurate simulation of the real measured DLTS spectra.

### Software environment

A software environment was created using MATLAB software package [10]. This solution included a so called graphic unit interface to ensure a user friendly environment, control and also a suitable graphic visualization. The interface (Fig.2) allows selecting the measured DLTS spectra and shows the basic measurement parameters (Fig.2, yellow rectangle), setting input parameters of the manual simulation (Fig.2, blue rectangle), calculating the automatic fitting parameters (Fig.2, purple rectangle), and it also shows the elapsed time with a graphic indicator (Fig.2, green rectangle). All the results are shown in the same graph indicated with different colors and marker types. The blue curve indicates the measured data, the green curve illustrates the manually added parameters simulation and the red one the result of the automatic fitting algorithm.



**Fig.2:** Software interface for managing the fitting process, coloured sections are the following: yellow – measurement data, green – process indicator, blue – manual fitting input data, purple – automatic fitting input data

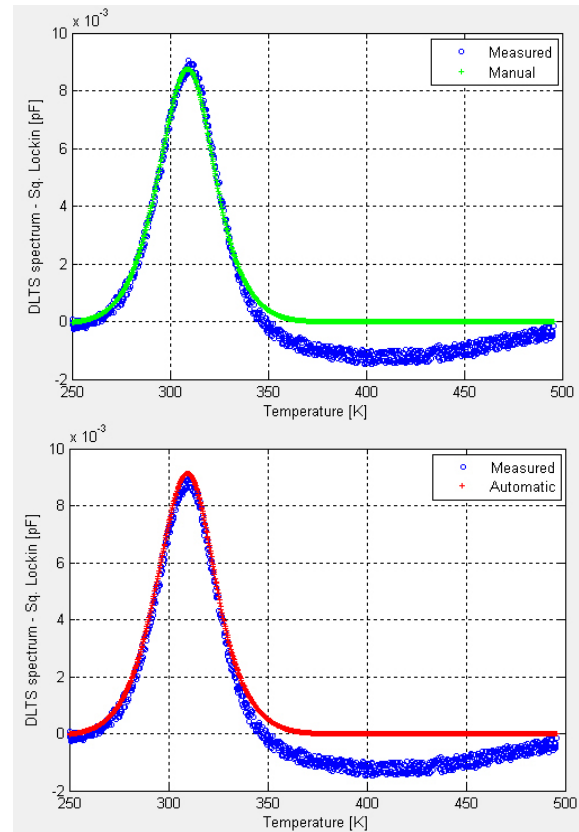
## RESULTS AND DISCUSSION

As fitting input of the simulations real measured DLTS spectra were used obtained by the measurement system DL 8000 DLTFs at our institute in Bratislava. The proposed algorithm was tested on measured data of a 4H-SiC radiation detector [11]. This choice was made due to a clear peak, with a significant amplitude and curve with a peak maximum at 309.1 K and amplitude of 9 fF (Fig.3 blue curve). This peak represents a definite defect state, which is suitable to test the accuracy and relevancy of the designed simulations. This measured result was evaluated using the measurement units' evaluation software with a so called "Direct evaluation" method. This means, that the calculation and evaluation of the Arrhenius curve was realized direct from the measured capacitance transients [9]. The obtained data via this evaluation, thus the activation energy 0.642 eV the capture cross section (Sigma)  $1.9 \times 10^{-15} \text{ cm}^2$  and the trap concentration  $6.49 \times 10^{11} \text{ cm}^{-3}$  (Tab. 1) were used to manually simulate the corresponding curve, which is labelled with green color on Fig.3. We can notice here a slight difference between the measured and the manually simulated data with an amplitude deviation of  $\Delta C = 0.3 \text{ fF}$  and temperature difference of  $\Delta T = 1.8 \text{ K}$  at peak maximum.

The presented software simulation that is the automatic fitting algorithm tries to overcome these differences by the designed software procedure described before. The elimination of the curve deviation, hence the usage of the proposed automatic algorithm, evoked an approximately identical curve in comparison with the measured one. The nearly perfect match between the measured and simulated data resulted also into the changes in the evaluated parameters (Tab. 1). These values (activation energy  $\Delta E_a = 0.627 \text{ eV}$ , sigma  $\sigma_n = 1.01 \times 10^{-15} \text{ cm}^2$ , trap concentration  $N_T = 6.76 \times 10^{11} \text{ cm}^{-3}$ ) showed the following changes between the trap parameters: energy  $\Delta E_a = 0.015 \text{ eV}$ , sigma  $\sigma_n = 0.89 \times 10^{-15} \text{ cm}^2$  and the trap concentration  $N_T = 0.27 \times 10^{11} \text{ cm}^{-3}$ . The simulated curve with the automatic method illustrated with red color is shown on Fig.3. The trap parameters calculated by the automatic fitting algorithm are listed in the purple coloured section of the interface shown on Fig.2.

**Tab. 1:** Comparison of the evaluated parameters and the results of the fitting algorithm of the DLTS spectra

	$\Delta E_a$ (eV)	$\sigma_n$ (cm <sup>2</sup> )	$N_T$ (cm <sup>-3</sup> )
Evaluated data by the DLTS measurement software	0.642	$1.90 \times 10^{-15}$	$6.49 \times 10^{11}$
Results obtained by the auto. simulation	0.627	$1.01 \times 10^{-15}$	$6.76 \times 10^{11}$
Delta differences	0.015	$0.89 \times 10^{-15}$	$0.27 \times 10^{11}$



**Fig.3** Result of the manual and automatic fitting algorithm

Differences between the evaluated data and the simulated ones (Tab. 1) are caused due to the fact that the DLTS measurement software calculates the trap parameters only by a specific number of measured capacitance transients. This number is defined by the evaluations input data, which only takes in account capacitance transients with a high exponential character. According to this the manually simulated curve has a shifted character with a different amplitude. The proposed approach, the automatic fitting algorithm calculates the trap parameters according to the DLTS spectrum character and thus ensures more precise curve and more precise values. The evaluated and calculated data with delta differences are shown in Tab. 1.

## CONCLUSION

The numerical fitting algorithm and the calculation of the parameters of deep energy levels were proposed and presented as an additional tool for the DLTS measurement evaluation. The fitting algorithm and the calculated data were tested and demonstrated using a 4H-SiC radiation detector [11]. The measured DLTS data were taken as an input curve, which was compared to the manually fitted curve where differences of 1.8 K in temperature, and 0.3 fF in amplitude at the peak maximum were obtained. The

numerical fitting process, especially the automatic fitting algorithm was able to generate more precise curve in comparison with the measured DLTS signal. According to the comparison of the manual and automatic method differences in energy  $\Delta E_a = 0.015$  eV, Sigma  $\Delta\sigma_n = 0.89 \times 10^{-15}$  cm<sup>2</sup> and the trap concentration  $\Delta N_T = 0.27 \times 10^{11}$  cm<sup>-3</sup> were obtained. Of course, the real nature of the fitted defect has to be checked using the physical model of the measured structure and also by reference data.

The execution of the presented fitting algorithm and the calculation of the deep energy level parameters can sometimes be time-consuming. The time needed for the fitting is relevant to several input parameters of the fitting algorithm: the shape of the measured DLTS curve, the size of the parameter ranges, the parameter step and precision. Careful setting of the input parameters may decrease the fitting time and still remain the same accuracy of the results. Before the fitting process user can simulate a spectrum using the manual module of the software environment and by several quick simulations the input parameters for the automatic simulation can be more precisely set.

The numerical fitting algorithm needs much more calibration and accuracy improvements which can be ensured by a further improvement of the interfaces instruction set. At last, but not the least, the physical interpretation of the simulated peaks needs to be integrated, so that the calculated peaks obtained by the fitting algorithm could be supported by the physical explanation of the deep energy level nature.

## ACKNOWLEDGEMENT

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