Deep levels model identification in semiconductor barrier structures

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Abstract. Semiconductor barrier structures are essential elements of modern integrated electronics. The band theory explains properties of barrier structures using deep levels in the semiconductor band gap. The relentless interest in studying the characteristics of deep levels is due to practical needs, ambiguous interpretations and scatters of experimental results obtained by different researchers. In order to increase the accuracy of the measurements, a modified capacitive deep-level transient spectroscopy technic has been developed. A mathematical model of the hardware transformations of the barrier structure capacitance transient signal is developed and provided in this article. The model considers the nonexponentiality of the capacitance transient and the spectrometer hardware transformations nonlinearity. There are the results of the deep levels experimental studies in silicon diodes and the model parametric identification. The technic makes it possible to reduce by five or more times the six-sigma confidence interval for the discrete deep level activation energy determining in comparison with the round robin test results of ASTM F978-02.

1. Introduction

The electronics industry actively uses semiconductor physics applications to assess the quality of semiconductor devices and integrated circuits. Deep level transient spectroscopy (DLTS) is one of these applications\textsuperscript{[1-5]}. It is based on the band theory of semiconductors and explains in particular the capture and emission processes of charge carriers (electrons and holes) from deep traps. Deep traps are trapping centers, the activation energy of which is more than 10\% of the semiconductor band gap. Deep traps may have different nature, and they cause deep levels in the band gap of the semiconductor. Depending on the origin of the deep trapping center, its influence on the properties of a semiconductor device can be positive or negative\textsuperscript{[6-11]}. Therefore, a lot of attention is paid to the study of the characteristics of deep centers by physicists in academic laboratories\textsuperscript{[12-16]} and technologists in factories producing semiconductor devices and integrated circuits\textsuperscript{[17, 18]}.

Since the appearance of the first publication by D. Lang, the industry standard on DLTS has been approved and the database of semiconductor defects has been created, despite existing problems with the interpretation of experimental data. Among the problems discouraging implementation of DLTS into the electronics industry, we should highlight the followings:

- the relatively low accuracy of the activation energy measurements of a defect in a bulk semiconductor while the band gap potentially may be tightly populated with deep levels. This circumstance complicates the identification of defects in production conditions if the
potential dependence of the deep level activation energy on the temperature and the relatively small non-destructive testing temperature range of semiconductor products is additionally taken into account. Also the so-called field effect diminishes the measurement accuracy [19];

- the position of the standard ASTM F978-02 regarding the determination of the second characteristic of the deep trap (the deep trap capture cross section) is not shared by all specialists in the field of DLTS;

- in addition to bulk defects with line energy spectra, industrial semiconductor devices may contain surface defects, the energy spectra of which are associated with technology deviations and are not available in specialized databases [20].

This article is devoted to proposals for solving the mentioned problems that discourage the implementation of DLTS into the semiconductor technology. To verify the proposals, the experimental studies were performed.

2. Methods

2.1. Method Description

We have designed the modified deep level transient spectroscopy technique. It is based on the recording of the capacitance transient parameters of a semiconductor diode caused by deep traps. The modification consists in the use of the frequency temperature scanning with the correlation processing of the capacitance transients using the hardware selector. The scan result (the frequency scan) at a fixed temperature of the test sample is displayed as the output voltage of the DLTS-selector vs the filling pulse repetition rate \( F_0 \). The deep level filling pulse repetition rate is set by the external program-controlled generator in the range from 0.25 Hz to 2.5 kHz and is displayed on a logarithmic scale. The frequency scanning is performed within the specified range with a step selecting by the operator of the control computer. The sensitivity of the capacitive bridge allows for the imbalance of ± 1 pF to get the signal with amplitude ± 10 V at the output of the synchronous detector. The measuring sinusoidal signal with the frequency of 1 MHz and the amplitude of 100 mV is applied to the sample. The circuit of the measuring capacitive bridge allows us to apply to the sample bias voltage pulses with the amplitude in the range from 0 to 12 V to fill and empty deep traps. The filling pulse length is 20 μs. To profile the distribution of deep traps in the differential mode (D-DLTS), it is possible to supply the second filling pulse synchronized with the negative half-period of the weighting function of the “lock-in” type selector.

2.2. Frequency scan model

If we assume that the depletion region is primarily in the low-doped material of the asymmetric diode and the majority carrier capturing by deep traps occurs in this area, we can determine the frequency scan model using well-known Laplace transforms as follows:

\[
S(\tau, C, F_0) = CK_{BS}K_{LS}\phi(\tau, F_0, t_1) \tag{1}
\]

where \( C \) is the amplitude of the capacitance transient, given in units of pF; \( K_{BS} = 10/B_S \) is the scale factor depending on the selected value of the total sensitivity \( B_S \) of the capacitive bridge with the output amplifier and the phase detector, which can be discretely selected from 1 pF to 1000 pF; \( K_{LS} = 10^4K_m/L_S \) is the selector scale factor, depending on its sensitivity \( L_S \), varying from 1 mV to 1000 mV; \( CK_{BS}K_{LS} \) is the amplitude of the transient signal at the output of the selector in units of V;

\[
\phi(\tau, F_0, t_1) = M\tau F_0\exp\left(-\frac{0.55}{\tau F_0}\right)\left[1 - \exp\left(\frac{t_1 F_0 - 0.45}{\tau F_0}\right) - \exp\left(-\frac{0.55}{\tau F_0}\right) - \exp\left(\frac{t_1 F_0 - 0.95}{\tau F_0}\right)\right] \tag{2}
\]

where \( \tau \) is the time constant of the capacitance transient of the deep trap; \( F_0 = 1/T_0 \) is the frequency of the weighting function; \( t_1 \) is the filling pulse length. The function \( \phi(\tau, C, F_0) \) has one maximum and tends to zero as \( F_0 \) tends to zero or infinity.

So that the output signal of the correlator does not depend on the factor \( M \), we normalize it as follows:

\[
S(\tau, C, F_0) = CK_{BS}K_{LS}\frac{\phi(\tau, F_0, t_1)}{K_m} \tag{3}
\]

where \( K_m = \max[\phi(\tau, F_0, t_1)] \) is the normalizing coefficient. It should also be the part of the \( K_{LS} \) scale factor characterizing the sensitivity of the selector so that the equation (1) does not change. The proposed
normalization, in the authors' opinion, allows, firstly, to simplify the determination of the scale factor \( M \) by including it in the \( K_{LS} \), and secondly, the ratio \( \varphi(\tau, F_0, t_1)/K_m \), as will be shown below, allows to take into account the nonexponentiality of the capacitance transient or the nonlinearity of the hardware selector and the phase detector at the output of the capacitive bridge.

To simultaneously take into account the nonlinearity of the hardware and the nonexponentiality of the capacitance transient, we determine a three-parameter mathematical model of the capacitance transient signal analog processing by the selector as follows:

\[
S(\tau, A, p, F_0) = A \left[ \frac{\varphi(\tau, F_0, t_1)}{K_m} \right]^p
\]

where \( A = CK_{BS}K_{LS} \), \( p > 0 \) is the coefficient that simultaneously carries information about the nonlinearity of the multiplier and the phase detector at the output of the capacitive bridge and about the nonexponentiality of the capacitance transient and other reasons, for example, different degree of the deep trap filling that is depending on the length of the filling pulse \( t_1 \). In this model, we suppose that the capacitance transient is caused by one deep level in band gap. To a first approximation, we can consider the phase detector and the analog multiplier connected in series a linear device with respect to the exponential output signal of the capacitive measuring bridge if the \( p = 1 \) and the deep trap filling is independent of the \( \tau \).

2.3. Experimental verification of the model

The experimental studies were performed on the silicon pulse diodes of the 1N4148 family from different manufacturers. The figure 1 shows two experimental frequency scans for different samples against the background of the models with three \( p \) values. The dashed lines against the background of the experimental points show the models. The samples differ in the levels of the capacitance transient signal against the background of the instrumental noise.

The parametric identification of \( p \) (see figure 1) can be performed on the full frequency scans by solving the inverse incorrect problem by minimizing the discrepancy (the standard deviation of the experimental data from the theoretical model) using various regularizations and convergence techniques. If for the first sample, to a first approximation, this procedure is not in doubt, then for the second sample, one should take into account the relatively large scatter of the experimental values at the low repetition rates of the deep trap filling pulses. In addition, for both samples, a careful examination of the behavior of the scans reveals deviations from the models when the output voltage of the selector changes. This circumstance has led us to the decision to study the behavior of the parameter \( p \) under the so called threshold identification.
The figure 2 shows the dependence \( p = f(k) \) for the sample № 3 at a constant temperature, where \( k \) is the threshold level of the scan, starting from which the higher part of the frequency scan participates in the parametric identification procedure. The constancy of the deep trap filling and emptying pulses voltages \( U_1 = -1 \) V and \( U_R = -12 \) V are also ensured. The \( k \) is set in fractions of the absolute value of the amplitude of the scan peak. The figure 3 shows the dependence \( p = f(T) \) for the constant values of \( k, U_1, U_R \).

\[
\begin{align*}
\text{Figure 2. The dependence } p = f(k), T = 253 \text{ K.} \\
\text{Figure 3. The dependence } p = f(T), k = 0.7.
\end{align*}
\]

The frequency scans of samples №4 (figure 4) and №5 (figure 5) differ significantly in shape from those shown in the figure 1 and need a separate interpretation. If the model in equation (3) can be separately applied for each peak of the sample №4, then for the sample №5 the scan model in equation (3) needs to be substantially adjusted.
3. Results and discussion

The figure 1 illustrates the increase in the accuracy of the modeling of the frequency scan by introducing the parameter $p$. The stronger signal (sample №1) corresponds to the parameter $1 \leq p \leq 1.5$, while the signal of the sample №2 is closer to the parameter $p=0.5$. Into the frequency scan model increases the accuracy of determining of the capacitance transient time constant $\tau$, which, together with a growth of the number of the experimental frequency scans, significantly increases the accuracy of determining of the activation energy of the deep trap $\Delta E$. In the experiment with 50 frequency scans in the temperature range from 262 K to 297 K, the relative accuracy of determining of the activation energy of the deep trap (three-sigma estimation) of about 2% was achieved. For comparison, according to the standard, the similar assessment of the accuracy of the determining of the deep trap activation energy according to the results of the inter-laboratory verification is about 5 times higher, that is, the accuracy of the determining of the deep trap activation energy in the standard is significantly lower.

The figure 2 shows an almost linear dependence of the parameter $p$ proposed by the authors on the threshold level $k$, which can be used for the additional identification of the deep level. In the figure 3, the dependence is not explicitly showed, which can be equally due to both the absence of the dependence and the insufficient accuracy of the signal measurements against the background of the instrumental noise.

Frequency scan in the figure 4, according to the authors, indicates the symmetric nature of the p-n junction and reflects the transient processes on both sides of the junction. Thus, using DLTS, it is possible to study the processes associated with the distribution of shallow traps. The model in equation (3) can be applied for each peak separately. To explain the results shown in the figure 5, the model in
equation (3) is unsuitable, since in all probability we are dealing with the combined influence of bulk and surface deep centers.

4. Conclusions
1. The introduction of the parameter $p$, which characterizes the nonexponentiality of the relaxation signal and the nonlinearity of the hardware, into the model of the frequency scan can significantly (5 or more times) increase the accuracy of the activation energy identification of the deep donor level in the low-doped n-type region of the diode. This circumstance will allow us to return to the idea of the interlaboratory verification at the new level of measurements.

2. The dependences of the parameter $p$ on the temperature of the sample and the threshold level of the scan relative to the peak amplitude in the future can become additional parameters in identifying a defective product and controlling manufacturing process instead of the deep-level capture cross-section.

3. The frequency scan allows in some cases to draw a conclusion about the degree of major impurities distribution asymmetry in the diode, which is the additional characteristic of the quality of the device.

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