COMPUTATIONAL APPROACH OF THE DARK CURRENT SPECTROSCOPY IN CCDs AS COMPLEX SYSTEMS. I. EXPERIMENTAL PART AND CHOICE OF THE UNIQUENESS PARAMETERS

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Dispozitivele cuplate prin sarcini (CCD) sunt sisteme complexe, chiar şi valabilitatea relaţiei Arrhenius şi a regulii Meyer-Neldel pentru CCD reprezentând "amprente" ale caracterului lor complex. În consecinţă, o abordare asistată de calculator a dependenţei de temperatură a curenţilor de întuneric (DTCI) din CCD necesită atât o alegere prealabilă riguroasă a parametrilor lor dominanţi de univocitate (PDU), cât şi un studiu amănunţit al compatibilităţii modelelor teoretice simplificate corespunzând acestor PDU relativ la datele experimentale existente. Pentru a obţine evaluări suficient de precise ale <u>mai multor</u> parametri fizici decât cei evaluaţi de metoda clasică a Spectroscopiei Curenţilor de Întuneric (DCS) în CCD, această lucrare a studiat detaliat atât procedura şi datele experimentale privind DTCI, cât şi cele mai bune posibilităţi de identificare a PDU.

The Charge Coupled Devices (CCDs) are complex systems, even the validity of the Arrhenius' relation and of the Meyer-Neldel rule for CCDs representing "fingerprints" of their complex character. For this reason, the computational approach of the temperature dependence of dark current (TDDC) in CCDs requires a previous suitable choice of their dominant uniqueness parameters (DUP), as well as a detailed study of the compatibility of the simplified theoretical model corresponding to these DUP with the existing experimental data. In order to obtain sufficiently accurate evaluations of <u>more</u> physical parameters than those given by the classical Dark Current Spectroscopy in CCDs, this work studied thoroughly both the experimental procedure and data referring to the TDDC in CCDs, as well as the most rigorous identification of the corresponding dominant uniqueness parameters.

Key words: Dark Current Spectroscopy, Charge Coupled Devices, Complex Systems, Dominant Uniqueness Parameters, Diffusion & Depletion Dark Current, Deep Traps Energies in Silicon, Capture Cross-Sections of electrons and holes.

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1. Introduction

A recent state-of art review of the Dark Current Spectroscopy (DCS) of CCDs [1] pointed out that this important method (for the identification and monitoring of even low impurity concentrations [2]) was thoroughly studied both from the point of view of the implied physical processes [3] – [5] and of the experimental (electronics) techniques [6] - [8], but … besides the general software tools used for the spectral analysis, the computational approach specific to this method seems to be almost completely missing. A unique example: the most accurate expression used for the evaluation of the (average) capture cross-section in the basic papers on DCS [7], [2], [1] seems to be that (relation (3) from page 719 of paper [7b]) referring to the spacing between 2 successive peaks (for N_t and N_t+1 traps of energy E_t) of the depletion dark current:

$$\text{Peak spacing} = n_i(T) \cdot V_{th}\sigma \cdot e^{-|E_t - E_i|/kT} \; .$$

Or, the comparison with relations (7'), (10), (10') and (11) of this work points out that besides the usual assumptions: $n, p << n_i$, the basic works on DCS in CCDs assume also that $|E_t - E_i| >> kT$ [7] or $E_t \cong E_i$ [2], $\sigma_p \cong \sigma_n$ [1], [2], [7], etc, hypotheses which are: a) obviously inexact, b) not necessary, as it results from the computational approach which follows, c) leading to inaccurate evaluations of the impurities parameters.

One finds that, due to their huge number of uniqueness parameters, of the involved microscopic transition processes, etc, the CCDs are complex systems [9], hence the computational approaches are absolutely necessary in order to: a) ensure the best possible accuracy of the numerical evaluations, b) provide numerical evaluations of more physical parameters (than the classical DCS works) of the impurified semiconductor, and ensure so: c) correct identifications and monitoring of impurities. Given being the multiple nonlinear terms involved by the classical theoretical (quantum) expression of the dark current in CCDs [3], the numerical evaluation of their parameters meets many computational problems, not at all easy to be solved, hence the use of the computational approach is necessary.

In order to achieve the statistical study of the compatibility of theoretical models corresponding to the chosen dominant uniqueness parameters with the experimental results, as well as of the convergence behavior of the successive approximations (iterative) procedure of the uniqueness parameters evaluation, a previous study of the used experimental method and the registration of the selected and studied experimental data is also necessary.

We have to mention also that the special interest shown in the behavior of CCDs at low temperatures is due to: a) the requirement to improve their quality (merit) factors, defined as:

$$Q = \frac{I_{photo-current}}{I_{dark\ current}}, \tag{1}$$

b) the quasi-exponential decrease of CCDs dark current at low temperatures (under 273 K). The last feature leads to very weak dark current at low temperature, e.g. – for different pixels of dimensions $24 \times 24\ \mu m$, at 222 K – we obtained values between 3×10^{-4} and 2.5×10^{-2} counts/s [10].

2. Experimental Part

2.1. The set-up and procedure used for the experimental determination of dark current in CCDs at low temperatures

(i) Camera

For the dark current study a backside illuminated SpectraVideo CCD camera manufactured by Pixelvision, Inc. in Beaverton, Oregon was used.

The camera system consisted of three parts:

1. A head assembly with sensor and cooling element,
2. A camera control box with the power supply and control boards to operate the mechanical shutter, the cooler, and clocking,
3. A data-acquisition board that received the image data from the control box and placed the pixel values into the PC memory.

The image sensor was a 512 x 512 SI003AB thinned CCD chip:

Image size	12.3 mm x 12.3 mm
Pixels	512 x 512
Pixel size	24 μm x 24 μm
Full well capacity	>300,000 electrons
Readout amplifier noise	5-8 electrons per readout at 228 K (-45°C)
Readout rate	500,000 pixels per second

(ii) Temperature adjustment and stabilization

The backside of the camera head is connected to a water-cooled Peltier element, which provides temperatures at the chip as low as 70 K below ambient temperature. The camera was very sensitive and showed an average increase in the count rate of about 5 counts/second with a closed shutter and with room lights on. Because the light leakage was through the shutter the camera cap was attached and additional coverings were added to prevent photons from reaching the sensor. The data was transferred via fiber optic cables from the control box to the data acquisition board in the PC. The camera came with an image acquisition and analysis software package (Pixelview) and a software developer kit. The software developer kit made it possible to control the camera by the use of Dynamic Link Libraries (DLLs). The temperature settings used were 223 K, 233 K, 243 K, 253 K, 263 K, 273 K, 283 K and 293 K but the measured temperature on the camera control box showed slightly different temperatures. The calibration was pre-adjusted from the manufacturer and was between 1 K and 2 K off. The actual temperatures on the chip, as given by the display on the control box, were given by 222 K, 232 K, 242 K, 252 K, 262 K, 271 K, 281 K and 291 K. At each temperature, pictures for 9 different exposure times were taken. 52 pictures were taken for each of the following exposure times: 3 sec, 5 sec, 10 sec, 20 sec, 50 sec and 100 sec and 22 images each for 250 sec and 500 sec and finally 12 pictures at 1000 sec. After setting the temperature the camera was stabilized for 2 hours. Then a series of dark exposures and bias frames were taken. The camera ran 13 hours for each temperature and the whole data set took 4 days and 8 hours to obtain. Each picture needed 1024 kB storage space on the hard disk and the whole data set of 5056 pictures used roughly 5 GB. By subtracting the subsequent bias frame from the raw dark frame picture, the “real” dark frame (thermal frame) was obtained.

2.2. Selected Experimental Results

We studied the dark current of 20 randomly distributed pixels for a backside-illuminated CCD housed in a Spectra Video camera (model SV512V1) manufactured by Pixelvision, Inc. The obtained results referring to the averaged (for each temperature, in the above indicated interval: 222…291 K) dark current and to their standard deviations (for each temperature and pixel) are indicated by Table 1.

3. Theoretical Part (the Main Sources of Dark Current)

The most important sources of dark current in a CCD are [3]: a) the diffusion dark current generated in the field-free region, b) the depletion (or bulk) dark current generated in the depletion region, and: c) the surface dark current generated at the Si-SiO_2 interface. If the CCD is operated in a multi-pinned phase (MPP) mode, then the interface is completely inverted with a high hole carrier concentration, hence the surface dark current from the Si-SiO_2 interface will be almost completely suppressed. The analysis of the diffusion and depletion dark current was achieved in the frame of various books on semiconductors, the more important being those of Grove [4] and Sze [5].

3.1. Diffusion dark current

Starting from the basic works [4], [5], the problem of the temperature dependence of the diffusion dark current was examined thoroughly in the frame of works [10], [11], being derived the expression:

$$De^{-}_{diff}(T) = De^{-}_{0,diff} \cdot T^{3} \exp\left(-\frac{E_g}{kT}\right), \tag{2}$$

where the diffusion pre-exponential factor is given by the relation:

$$D_{0,diff}^{-} = \frac{D_n A_{pix} c_n^2}{x_c \cdot N_A} \ . \tag{3}$$

Table 1

Dark Current and their associated standard deviations (counts/s) in CCDs for 20 randomly selected pixels [5b] (obtained by a linear fit to exposure times from 3 s to maximum 100 s)

Coordinates of the pixel	Dark currents/their standard deviations (counts/s) at temperature (K)							
	222	232	242	252	262	271	281	291
41, 120	0.001484 0.003801	0.026228 0.004092	0.100662 0.004996	0.424933 0.005074	1.969514 0.009783	9.228712 0.024020	44.35249 0.116985	217.7895 0.759432
61, 140	0.012969 0.003071	0.040539 0.003757	0.149438 0.005368	0.618415 0.006873	2.505146 0.008665	10.75346 0.028474	48.04459 0.114976	227.3067 0.647973
81, 160	0.008295 0.003253	0.034914 0.003672	0.129242 0.004039	0.526984 0.005315	2.218795 0.011491	9.733896 0.025364	45.19955 0.113001	219.0285 0.725327
101, 180	0.006282 0.002548	0.023767 0.002857	0.095945 0.004635	0.415553 0.005956	1.880534 0.010914	8.843086 0.015512	43.17259 0.132231	214.2660 0.613028
121, 200	0.006063 0.004052	0.029031 0.002548	0.112173 0.005572	0.474378 0.006013	2.053744 0.008049	9.471216 0.023343	44.65022 0.121548	216.9518 0.670435
141, 220	0.008583 0.005063	0.026559 0.003158	0.102486 0.003196	0.440118 0.006127	1.941113 0.011376	9.129981 0.021374	43.64158 0.125649	215.0924 0.668302
161, 240	0.005350 0.003870	0.023663 0.003731	0.093614 0.005877	0.428868 0.004603	1.981857 0.011907	8.892988 0.020439	43.45940 0.130858	215.9305 0.566935
181, 260	0.006074 0.001499	0.022282 0.003255	0.091008 0.003704	0.398030 0.004488	1.838440 0.010817	8.730706 0.23186	42.30294 0.103747	211.0063 0.573907
201, 280	0.017147 0.003917	0.065254 0.003527	0.234979 0.004027	0.868245 0.005721	3.188347 0.014037	12.20961 0.021103	52.23446 0.132068	237.3687 0.691883
221, 300	0.015157 0.002669	0.053210 0.004043	0.189289 0.005228	0.730125 0.006754	2.798395 0.012475	11.44398 0.024583	49.53068 0.132898	229.4021 0.618210
241, 320	0.006311 0.003286	0.033265 0.004260	0.123681 0.005276	0.501478 0.006200	2.086141 0.009312	9.464486 0.026488	44.62626 0.117747	217.6235 0.770354
261, 340	0.012803 0.002676	0.057419 0.004590	0.210351 0.006103	0.818504 0.006205	3.116074 0.012573	12.01514 0.022625	51.54383 0.110135	236.1418 0.698540
281, 360	0.018370 0.004135	0.072716 0.003395	0.253919 0.005953	0.967605 0.007893	3.481746 0.014576	13.30162 0.027987	54.33791 0.117103	242.3072 0.707761
301, 380	0.014709 0.004061	0.060266 0.003328	0.218637 0.004604	0.812199 0.006859	3.061305 0.010382	12.36033 0.026695	53.08315 0.131517	243.6041 0.660860
321, 400	0.003675 0.003399	0.007298 0.002638	0.039933 0.004259	0.244118 0.005207	1.421787 0.009869	7.927352 0.022172	41.07097 0.122311	209.9430 0.644753
341, 420	0.012025 0.004043	0.051089 0.004244	0.196514 0.004187	0.777152 0.005926	2.943100 0.012192	11.37274 0.024829	49.31115 0.091369	231.6490 0.645724
31, 247	0.025084 0.003162	0.084750 0.003970	0.316796 0.005551	1.129892 0.007459	3.855564 0.017382	12.72840 0.029811	51.63198 0.104765	234.6485 0.648644
29, 88	0.009511 0.003712	0.041729 0.004608	0.161847 0.003975	0.647090 0.006759	2.568672 0.013650	10.73541 0.023608	47.82530 0.123029	226.2279 0.683945
188, 471	0.005372 0.003983	0.017136 0.003858	0.074848 0.005254	0.365805 0.006436	1.818186 0.011591	9.043002 0.019539	44.73338 0.136305	223.1231 0.685422
161, 289	0.000314 0.003930	0.002851 0.003629	0.021359 0.004255	0.171535 0.005205	1.154768 0.011748	6.980657 0.023886	37.94227 0.109691	199.2435 0.574439

The physical meanings and the numerical values of the parameters implied in the expression (3) were estimated also in the frame of study [10b], namely:

(i) D_n (the diffusion coefficient) $\cong 25\, cm^2/s$, for silicon,

(ii) $$c_n = \sqrt{N_v N_c} \cdot T^{-3/2} = 2\left(\frac{2\pi k}{h^2}\right)^{3/2} \cdot m_e^{3/4} \cdot m_h^{3/4} \cong 3.284 \times 10^{15} cm^{-3} \cdot K^{-3/2}, \quad (4)$$

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where N_v, N_c are the effective densities of the quantum states in the valence and conduction bands, respectively, while m_e, m_h are the effective masses of electrons and holes, respectively,

(iii) N_A is the concentration of the acceptor impurities $\approx 4 \cdot 10^{14} cm^{-3}$,

(iv) $A_{pix} \approx 5.76 \times 10^{-10} m^2$ is the area of a pixel, while:

(v) x_c is *the characteristic length of the diffusion process*, whose value can be determined starting from the above indicated values and the measured diffusion pre-exponential factor $De^-_{0,diff}$, the obtained value being: $x_c \approx 27\ \mu m$.

3.2. The depletion dark current

According to the theoretical model of Hall [3b], Shockley and Read [3a], the contribution of the depletion processes to the dark current is given by the expression:

$$De^-_{HSR} = -\frac{x_{dep} \cdot n_i^2 \cdot A_{pix}}{U}, \quad (5)$$

where the net generation-recombination rate U corresponding to the impurities and/or imperfections of the semiconductor lattice is described by the relation[5]:

$$U = \frac{\sigma_p \sigma_v V_{th}\left(n \cdot p - n_i^2\right) N_t}{\sigma_n \left[n + n_i \exp\left(\frac{E_t - E_i}{kT}\right)\right] + \sigma_p \left[n + n_i \exp\left(\frac{E_i - E_t}{kT}\right)\right]}. \quad (6)$$

In the above expression, σ_p, σ_n are the capture cross-sections for holes and electrons, respectively, V_{th} is the thermal velocity, E_i is the intrinsic Fermi energy level, N_t is the concentration of traps, i.e. of bulk generation-recombination centers at the energy level E_t, while n, p, and n_i are the electrons,

[5] At thermal equilibrium: $n \cdot p = n_i^2$, hence $U_{dep} = 0$ (the recombination and generation rates being then equal).

the holes and the intrinsic carrier concentration, respectively, given by the expressions: $n = 2\left(\frac{2\pi \cdot m_n kT}{h^2}\right)^{3/2} \exp\frac{\mu - E_c}{kT}$, $p = 2\left(\frac{2\pi \cdot m_p kT}{h^2}\right)^{3/2} \exp\frac{E_v - \mu}{kT}$, (7)

$$n_i = 2\left(\frac{2\pi\sqrt{m_n m_p} \cdot kT}{h^2}\right)^{3/2} \cdot \exp\left(-\frac{E_g}{2kT}\right) = c_n(T) \cdot T^{3/2} \cdot \exp\left(-\frac{E_g}{2kT}\right), \qquad (7')$$

where m_n, m_p are the effective masses of the free electrons and holes, respectively, E_c, E_v, μ, and E_g are the lower/higher threshold of the conduction/valence band, respectively, the electrochemical potential and the energy gap of the considered semiconductor, respectively, which are also temperature dependent.

Taking into account the relations (5) - (7'), it results that the temperature dependence of the depletion dark current given by the Hall-Shockley-Read theoretical model can be written as:

$$De^-_{dep}(T) = De^-_{0,dep} \cdot T^{3/2} \cdot \exp\left(-\frac{E_g}{kT}\right), \qquad (8)$$

where $De^-_{0,dep}$ is the *effective* depletion pre-exponential factor.

4. Numerical Modeling

From relations (2) - (7'), it results that the numerical description of the temperature dependence of the dark current in CCDs requires a huge number of uniqueness parameters: $D_n, x_c, A_{pix}, N_A, m_e, m_h$, $E_g, x_{dep}, n_i, \sigma_p, \sigma_n, V_{th}, N_t, n, p$, $|E_t - E_i|$, etc, many of them [e.g. *n, p,* n_i, etc, as it results from relations (7), (7')] being also temperature dependent, hence introducing some additional uniqueness parameters [as μ, E_c, E_v, etc which are also temperature dependent, implying other uniqueness parameters, and so on].

One finds so that the description of the temperature dependence of the dark current in CCDs requires also: a) some simplifications of the rigorous quantum mechanics Hall-Shockley-Read model, (ii) some numerical descriptions of the temperature dependence of some uniqueness parameters (as the energy gap E_g), (iii) an ordering of the uniqueness parameters upon their influence on the dark current values and a convenient choice of a limited number of uniqueness parameters, which can describe accurately the dark current in CCDs.

4.1. The approximation of the completely depleted zone

Assuming that in the depletion zone, the electric field sweeps the holes to the *p*-substrate and the electrons to the potential wells, hence (in this region):

$n, p << n_i^2$, the temperature dependence of the depletion dark current will be described – for a single species of deep-level impurity - by the expression [see relations (5) and (6)]:

$$De_{HSR}^{-} = \frac{x_{dep} A_{pix} n_i \left[\sigma_n \exp\left(\frac{E_t - E_i}{kT} \right) + \sigma_p \exp\left(\frac{E_i - E_t}{kT} \right) \right]}{\sigma_p \sigma_v V_{th} N_t} . \qquad (9)$$

It results that the relation (9) can be written in the equivalent form:

$$De_{dep}^{-} \equiv De_{HSR}^{-} = De_{0,dep}^{-} \cdot T^{3/2} \cdot \exp\left(-\frac{E_g}{2kT} \right) \cdot \sec h\left[\frac{E_t - E_i}{kT} + d \right], \qquad (10)$$

where the depletion pre-exponential factor is given by the expression:

$$De_{0,dep}^{-} = \frac{x_{dep} A_{pix} c_n \sqrt{\sigma_p \sigma_n} \cdot V_{th} N_t}{2} , \qquad (10')$$

and "*the polarization degree" d of the capture cross-sections for electrons and holes, respectively*, is:

$$d = \arg\tanh\left(\frac{\sigma_n - \sigma_p}{\sigma_n + \sigma_p} \right) . \qquad (11)$$

If several impurity species $j = 1, N_i$ are present for the studied pixel, then the total dark current will be [see relations (2), (7'), (10) and (10')]:

$$De^{-}(T) = De_{0,diff}^{-} \cdot T^3 \exp\left(-\frac{E_g(T)}{kT} \right) +$$

$$+ \frac{x_{dep} A_{pix} V_{th}}{2} \cdot c_n(T) \cdot \exp\left[-\frac{E_g(T)}{2kT} \right] \cdot \sum_{j=1}^{N_i} \sqrt{\sigma_{pj} \sigma_{nj}} \cdot N_{tj} \cdot \sec h\left[\frac{E_{tj} - E_i}{kT} + d_j \right]. \qquad (12)$$

Given being the very large number of uniqueness parameters involved by the expression (12), the introduction of some *effective parameters* as the effective energy gap $E_{g,eff.}$, the effective average capture cross-section $\sigma_{eff} = \sqrt{\sigma_{p,eff.} \sigma_{n,eff.}}$, the effective deep-level traps energy $E_{t,eff}$, and the effective polarization degree of capture cross-sections d_{eff} (denoted in following by E_g, $\sigma \equiv \sqrt{\sigma_p \sigma_n}$, E_t and d) has to be used by equating (by means of some averages over temperatures and impurities, respectively) in computations the detailed expression (12) with the sum of expressions (2), (10) [the last one involving the relation (10')]. Due to these concomitant averages, all effective parameters [the effective energy gap: $E_{g,eff.}$ (denoted in following by E_g for simplicity), inclusively] will have values dependent on the studied pixel.

Assuming equal capture cross-sections for holes and electrons, hence a null polarization degree, the expression of the temperature dependence of the depletion dark current becomes:

$$De_{dep}^{-} \equiv De_{HSR}^{-} = De_{0,dep}^{-} \cdot T^{3/2} \cdot \exp\left(-\frac{E_g}{2kT}\right) \cdot \sec h\left[\frac{E_t - E_i}{kT}\right]. \qquad (10")$$

Because the temperature dependence of all physical parameters of the pre-exponential factor seems to be very weak (in comparison with the exponential dependence of the last 2 factors, especially), we can assume that the temperature dependence of the depletion dark current is due mainly to the last 3 factors of expression (12).

The next matter of our study will refer to the evaluation of the magnitude order of temperature dependence of the true energy gap $E_g(T)$, because this parameter is involved by the strongest exponential functions of the 2 terms of relation (12).

4.2. Basic features of the most efficient generation-recombination traps

As it is well known (see e.g. [4], [5], [10]), the effective generation-recombination life of electrical charge carriers in the depletion region is defined and expressed as:
$$\tau \overset{\Delta}{=} \frac{n_i}{2U} = \frac{x_{dep} A_{pix} n_i}{2De_{dep}^{-}} = \frac{\sigma_n \exp\left(\frac{E_t - E_i}{kT}\right) + \sigma_p \exp\left(\frac{E_i - E_t}{kT}\right)}{\sigma_p \sigma_v V_{th} N_t} \ . \qquad (13)$$

It is very easy to find that this effective generation-recombination life presents a sharp minimum (i.e. a maximum dark current emission) for:

$$0 = \frac{d\tau}{dE_t} = \frac{1}{\sigma_p \sigma_n V_{th} N_t}\left[\frac{\sigma_n}{kT} \exp\frac{E_t - E_i}{kT} - \frac{\sigma_p}{kT} \exp\frac{E_i - E_t}{kT}\right], \qquad (14)$$

equivalent to the condition:
$$E_t = E_i + \frac{kT}{2} \ln\left(\frac{\sigma_p}{\sigma_n}\right). \qquad (14')^6$$

In the studied scientific literature [1], [2], [7], there are reported the values: a) $|E_t - E_i| \leq 30\, meV$, for Ni, Co, Mo and a first trap Au_1, b) $\leq 50\, meV$ for Mn, c) $\approx 60\, meV$ for Pt, d) $120...150\, meV$ for Fe_1, and: e) 100…270 meV for 3 traps of unknown nature.

Because in the middle of the temperature interval studied by us (≈ 260 K), we have: $\frac{kT}{2} \cong 11.2125\, meV$, it results that: (i) $|E_t - E_i| / (E_g/2) \leq 0.2$, hence the most active impurities correspond to a rather deep energy levels (near to the Fermi level, i.e. they correspond to *deep-level traps*),

6 From relations (14), (14'), it results also that: a) if the deep-level trap is located (slightly) above the intrinsic Fermi level, then the capture cross-sections of holes will be prevail to those for electrons, b) conversely, if this trap is located (slightly) below the intrinsic Fermi level, then the capture cross-section of electrons will prevail, but – at least, for moment – these features cannot be detected using only the temperature dependence of dark current.

(ii) $|E_t - E_i|/(kT/2) \cong 2...10$, it results that the polarization degree of the capture cross-sections of holes and electrons, respectively, has to be rather large (larger than 1, hence considerably different than 0).

From the condition (14), it results that at exactly the maximum emission of the depletion dark current:

$$d = \frac{1}{2}\ln\left(\frac{\sigma_p}{\sigma_n}\right) = \frac{|E_t - E_i|}{kT}, \qquad (15)$$

hence then the terms of the hyperbolic secant (sech) are exactly equal.

It results that in such conditions, the magnitude order of the polarization degree d will be the same as that of $|E_t - E_i|/(kT/2)$, i.e. values of the magnitude order of 2…10.

Of course, the experimentally found depletion dark current do not correspond exactly to the emission maximum, hence: a) some specific numerical calculations are necessary, but: b) the assumption on the possibility to consider the capture cross-sections of holes and electrons as equal seems to be wrong.

4.3.The temperature dependence of the silicon energy gap

In the frame of our study, we met 2 types of temperature dependencies of the silicon energy gap: a) *the linear dependence* implicitly existent in the experimental data reported by Grove [4]: $E_g(eV) = a + b \cdot T \cong 1.2 - 3.4\times10^2 T$, (16)

and: b) *the non-linear dependence* reported by Varshni [12] and Sze [5]; according to [12], for the most semiconductors: $E_g = E_{g0} - \alpha \cdot T^2/(T+\beta)$, (17)

the values of the new uniqueness parameters being for pure silicon [5]:

$$E_{g0} \approx 1.17\ eV,\ \alpha \approx 4.73\times10^{-4}\ K^{-2},\ \beta \approx 636\ K.$$

It is very easy to find that:

a) for the linear temperature dependencies (of Grove's type), the linear term $b \cdot T$ will "glide" from $\exp(-E_g/2kT)$ in the depletion pre-exponential factor, whose expression becomes: $De_{0,dep}^{-} = \frac{x_{dep} A_{pix} c_n \sqrt{\sigma_p \sigma_n} \cdot V_{th} N_t}{2} \cdot \exp\left(\frac{b}{k}\right)$, (18)

b) the Sze's expression (14) can be written in the equivalent forms:

$$\text{(i)}\quad E_g(eV) \cong 1.17 - \frac{4.73\times10^{-4} T^2}{T+636} \cong 1.471 - 4.73\times10^{-4} T - \frac{191.3266}{T+636}, \qquad (17')$$

and – because the range of the studied temperatures 222…291 K corresponds approximately to the interval $893 + \Delta T$, where $\Delta T \in (-35, +35) K$:

$$\text{(ii)}\quad E_g(eV) \cong 1.256 - 4.73\times10^{-4} T + 0.21425\left[\frac{\Delta T}{893} - \frac{(\Delta T)^2}{893^2}\right], \qquad (17'')$$

the "amplitude" of the last term (the non-linear one) being of only 0.329 meV.

Because the magnitude order of the modulus $|E_t - E_i|$ was found as considerably larger: 10…270 meV, it results that – in first approximation – we can neglect the temperature dependence of the silicon energy gap.

We will mention also that the work [2] uses a fix (effective, i.e. temperature independent) value of the energy gap of silicon equal to $E_g = 1.08\, eV$.

4.4. Choice of the uniqueness parameters

From relations (2), (10), it results that the most suitable expression of the temperature dependence of the dark current in CCDs is given by the relation:

$$\bar{De}(T) = \bar{De}_{diff}(T) + \bar{De}_{dep}(T) = T^3 \exp\left(\ln \bar{De}_{0,diff} - \frac{E_g}{kT}\right) + T^{3/2} \cdot \exp\left(\ln \bar{De}_{0,dep} - \frac{E_g}{2kT}\right) \cdot \operatorname{sech}\left[\frac{E_i - E_t}{kT} + d\right], \quad (19)$$

hence the most convenient choice of the uniqueness parameters corresponds to the order: a) $\ln \bar{De}_{0,diff}$, $\ln \bar{De}_{0,dep}$ (logarithms of the pre-exponential factors of the diffusion and depletion current, respectively) and E_g (the effective energy gap; see paragraph 4.1), b) the difference $E_t - E_i$ of the energies of the trap and of the intrinsic Fermi level, respectively, or its modulus $|E_t - E_i|$ [when the fitting relation (12) is used], c) the depolarization degree d of the capture cross-sections of electrons and holes, respectively, given by relation (11).

5. Conclusions

The accomplished study:

a) allowed a convenient choice of the most efficient 5 uniqueness parameters intended to some numerical descriptions, starting from the analysis of the temperature dependencies of many theoretical uniqueness parameters; all these results are supported also by the previously reported findings in the specialty literature (see [1] – [12]),

b) pointed out that unlike the classical papers [2], [7] of the DCS method which assume (and use for the evaluation of the effective capture cross-section $\sigma = \sqrt{\sigma_n \sigma_p}$) that the impurities (traps) contribution to the depletion dark current is described by an exponential function, the true (accurate) description is given by an exponential hyperbolic cosine [see relation (10)]; taking into account that $|E_t - E_i|$ is of the magnitude order of 1 or even larger, the corresponding systematic errors introduced here have the magnitude order of 50% or even larger (if $|E_t - E_i| > kT$),

c) pointed out that the argument of the hyperbolic cosine function involves a function (named by us polarization degree of capture cross-sections) of the difference $\sigma_n - \sigma_p$, whose numerical determination allows the evaluation of both capture cross-sections: σ_n, σ_p of the free electrons and holes, respectively,

d) pointed out that because all basic papers on the DCS method identify some pixels with only one type of impurities and even with only one trap/pixel, the above findings can be effectively applied for the accurate evaluation of both capture cross-sections σ_n, σ_p of the identified impurities,

e) pointed out that the numerical fit of the experimental data by the relation (10) allows accurate separate (discriminated) evaluations of both total diffusion and depletion current at all studied temperatures.

Some detail aspects of the computational approach of the method of Dark Current Spectroscopy (DCS) will be examined by the next issues of this series.

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