# COMPUTATIONAL APPROACH TO DARK CURRENT SPECTROSCOPY IN CCDs AS COMPLEX SYSTEMS. II. NUMERICAL ANALYSIS OF THE UNIQUENESS PARAMETERS EVALUATION

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*Datorită: a) numărului considerabil de parametri de intrare, b) relațiilor teoretice puternic neliniare (exponențiale), programele de calcul elaborate (pentru fitarea parametrilor de univocitate ai dependenței de temperatură a curenților de întuneric ai unor dispozitive CCD) sunt foarte sensibile la alegerea: (i) aproximațiilor de ordinul zero ale lățimii efective a benzii interzise a Si, (ii) ponderilor valorilor experimentale ale curenților de întuneric. Acest lucru conduce la: a) intervale înguste ale domeniilor de stabilitate ale aproximațiilor de ordinul zero care conduc la atractori cu semnificație fizică, înconjurate de: b) domenii conducând la oscilații, c) instabilități sau: d) pseudo-convergență (atractori falși, cu valori fără semnificație fizică ale parametrilor studiați), aspecte studiate în detaliu de această lucrare.*

*The evaluation of the uniqueness parameters of the temperature dependence in CCDs is difficult to the considerable number of input parameters and to the strongly nonlinear (exponential) theoretical relations. For this reason, the elaborated computer programs are very sensitive to the choice of the zero-order approximations of the effective (Si) energy gap, and of the weights associated to the experimentally determined dark current. The main goal of this work was to study the rather narrow stability domains of the zero-order approximations, which lead to attractors with physical meaning. It was found that the stability domains are surrounded by (usually in this order): other fields leading to oscillations, pseudo-convergence (false attractors, described by non-physical values of the studied parameters) or instability fields, which were studied also in detail.*

**Keywords:** charge coupled devices, attractors, stability domains, compatibility of theoretical models relative to experimental results, dark current, intrinsic fermi level, deep traps in silicon, capture cross-sections.

## 1. Introduction

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In the frame of our previous study [1], we have found that the minimal set of uniqueness parameters which ensure a sufficiently accurate description of the temperature dependence of the dark current in CCDs corresponds to: a) the logarithms of the pre-exponential factors $\ln De^-_{0,diff}$, $\ln De^-_{0,dep}$ of the diffusion and depletion dark current, respectively, b) the energy gap $E_g$ of silicon, c) modulus $|Et\text{-}Ei|$ of the difference of energies corresponding to the capture traps (of free electrons or holes) inside Si, and to the: d) so-called "polarization degree" $d$ of the capture cross-sections of free electrons $\sigma_n$ and holes $\sigma_p$, defined as:

$$d = \arg\tanh\left(\frac{\sigma_n - \sigma_p}{\sigma_n + \sigma_p}\right). \tag{1}$$

This work studied the obtained results concerning the uniqueness parameters of the CCD semiconductor: $\ln De^-_{0,diff}$, $\ln De^-_{0,dep}$, $E_g$ and $|E_t - E_i|$ by means of the classical gradient method [2]. In this aim, the expression of the total dark current (with the role of "tested" parameters $\bar{t}$ here) was written as (see [1], [3]):

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

$$+ T^{3/2} \cdot \exp\left(\ln De^-_{0,dep} - \frac{E_g}{2kT}\right) \cdot \sec h\left[\frac{E_t - E_i}{kT}\right]. \tag{2}$$

As it is known, the gradient method aims to find the values of the effective uniqueness parameters (described by the vector $\bar{u}$), by minimization of the sum $S$ of weighted deviations squares of the calculated values $\bar{t}_{calc}(\bar{u}, \bar{p})$ relative to their experimental values $\bar{t}_{exp}$: $S = \sum_{i=1}^{N} W_i(t_{calc.i} - t_{exp.i})^2 = (\bar{t}_{calc.} - \bar{t}_{exp.})^T \cdot \overline{\overline{W}} \cdot (\bar{t}_{calc.} - \bar{t}_{exp.})$,

$$\tag{3}$$

where $(\bar{t}_{calc.} - \bar{t}_{exp.})^T$ is the transposed of the difference of column vectors $\bar{t}_{calc.}, \bar{t}_{exp.}$, while $\overline{\overline{W}}$ is the diagonal matrix of weights.

The vector $\bar{C}^{(I)}$ of the correction of the vector $\bar{u}$ of uniqueness parameters in a certain successive approximation (iteration) $I$ is obtained by the condition to minimize the sum $S$ (if the functions $\bar{t}_{calc}(\bar{u}, \bar{p})$ would be linear):

$$\left[\frac{\partial(S^{(I)} + \delta S)}{\partial(\delta\bar{u})}\right]_{\delta\bar{u} = \bar{C}^{(I)}} = 0. \tag{4}$$

Due to the strongly nonlinear (exponential) character of the expression (2), the relation (4) does not lead always to the sum $S$ decrease, i.e. in some conditions it is possible to appear oscillations of positive and negative values of its change $\delta S$, or even some monotonic increases $\delta S > 0$. One finds so the appearance of

some numerical phenomena [4], the most important ones being: a) *the stable oscillations,* which are located in the field of values of physical meaning, but offer only some intervals of values, and not exact (effective) values of the studied uniqueness parameters, b) *the instability*, if this algorithm leads to some diverging results (obviously, without any physical meaning), and even: c) *the pseudo-convergence*, if the results given by the computer program converge, towards certain numerical values without physical meaning (see Fig. 1).

For this reason, we will examine below:

(i)    the statistical criteria used to study the compatibility of the theoretical model relative to the considered experimental data,

(ii)    the main specific criteria for the identification of the pseudo-convergence,

(iii)the choice of the zero-order approximations, extremely important because - due to the strongly nonlinear character of relation (2) – the stability domain could be rather narrow.
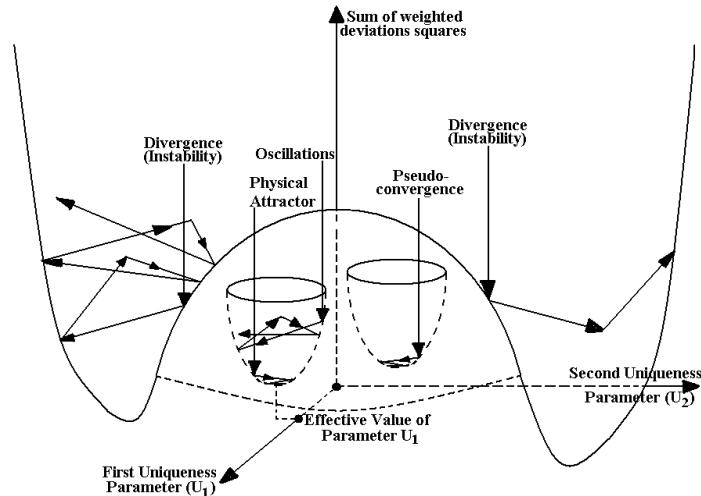


Fig. 1. Basic types of domains in the space of uniqueness parameters

## 2. Preliminaries of uniqueness parameter evaluation

**2.1. Preliminary evaluations of the zero-order approximations of the uniqueness parameters. Prediction possibilities of the convergence behavior of the evaluation process.**

It is known that at the limit of the lowest studied temperatures (222 … 242 K), and at that of highest temperatures (271 … 291 K), the diffusion process and the depletion one are prevalent, respectively [3] (see also Fig. 2). For this reason, it is possible to obtain some rough zero-order approximations of the uniqueness parameters starting from the linearization of the theoretical relation (2) at these limits. In this aim, we

will observe that if - condition fulfilled for some pixels, see Table 1: $| E_t - E_i | >> \dfrac{kT}{2} \approx 12 \; meV$ , then:

$$\exp\left(-\frac{|E_t - E_i|}{kT}\right) << \exp\left(\frac{|E_t - E_i|}{kT}\right) \; \text{and:} \; \cosh\left(\frac{|E_t - E_i|}{kT}\right) \approx \frac{1}{2}\exp\left(\frac{|E_t - E_i|}{kT}\right).$$

In such cases, the relation (2) can be well approximated by the expression :

$$De^-(T) = De^-_{0,diff} \cdot T^3 \exp\left(-\frac{E_g}{kT}\right) + 2De^-_{0,dep} \cdot T^{3/2} \cdot \exp\left(-\frac{1}{2kT}\Big[E_g + 2|E_t - E_i|\Big]\right). \; (2')$$
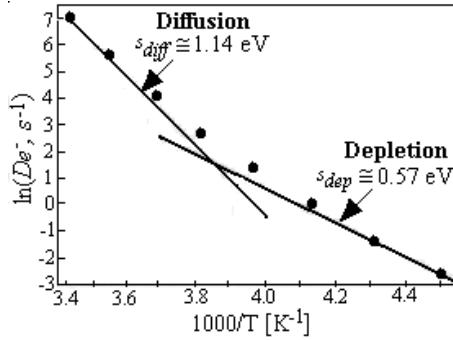


Fig. 2. Average of the dark current logarithm vs the inverse of temperature (see also [3b], fig. 5)

Assuming that the diffusion process is prevalent at higher temperatures (271…291 K):  $De^-(271...291\,K) \cong De^-_{diff} = De^-_{0,diff} \cdot T^3 \exp\left(-\dfrac{E_g}{kT}\right),$        (5)

and the depletion one prevails at lower temperatures (222…242 K):

$$De^-(222...242\,K) \cong De^-_{dep} \cong 2De^-_{0,dep} \cdot T^{3/2} \cdot \exp\left(-\frac{1}{2kT}\Big[E_g + 2|E_t - E_i|\Big]\right) ,$$        (6)

these expressions can be linearized as it follows :

$$\ln De^-(271...291\,K) \cong c_{diff} - s_{diff} \cdot \frac{1}{T} , \quad \ln De^-(222...242\,K) \cong c_{dep} - s_{dep} \cdot \frac{1}{T} \; . \; (7)$$

It results that some rough evaluations of the zero-order approximations of the uniqueness parameters of the temperature dependence of the dark current of CCDs can be obtained starting from the crossing-points coordinates $c_{diff}, c_{dep}$ and the slopes $s_{diff}, s_{dep}$ of the diffusion and depletion prevalence domains, respectively:

$$\ln De^-_{0,diff} \cong c_{diff} - 3\cdot \ln \widetilde{T}_{diff} , \quad \ln De^-_{0,dep} \cong c_{dep} - \frac{3}{2}\ln \widetilde{T}_{dep} - \ln 2 ,$$        (8)

and:        $E_g^{(0)} \cong -s_{diff} \cdot k , \quad |E_t - E_i|^{(0)} \cong \left(2s_{diff} - s_{dep}\right)\cdot k ,$        (9)

where $\tilde{T}$ is the average value of the 2…3 temperatures taken into considerations at each end of the $\ln De^- = f(1/T)$ plot.

From relations (6), (7), it results also that:

$$\frac{s_{diff}}{s_{dep}} \cong \frac{2}{1+2\left|E_t - E_i\right|/E_g} \ . \tag{10}$$

Taking into account that the values of the ratio $2\left|E_t - E_i\right|/E_g$ are involved in the range 0.0125 … 0.2 (see e.g. Table **1**), and that the prevalence of the diffusion and depletion dark current, at higher and lower temperatures, respectively, are not absolutely ones, it results that the ratio of the slopes $s_{diff}, s_{dep}$ is somewhat less than the value predicted by relation (10). One finds we can expect the following convergence behaviors of evaluation process:

$$\frac{s_{diff}}{s_{dep}} = \begin{cases} around\ of\ 1 \quad \rightarrow \quad instability,\ due\ the\ disagreement\ with\ the\ HSR\ results, \\ between\ 1.6\ and\ 1.95 \quad \rightarrow \quad convergence\ to\ an\ attractor\ with\ physical\ meaning \\ around\ of\ 2 \quad \rightarrow \quad instability\ or\ pseudo-convergence\ for\ E_{g0} > true\ E_g\ value \end{cases} \tag{11}$$

In order to check these predictions, Table 1 presents some selected results obtained by means of the above algorithm for different datasets leading to typical convergence behavior: a) physical convergence, b) pseudo-convergence (towards values without physical meaning), c) instability. One finds that sometimes (e.g. for pixel 61, 140) it is necessary to take into account at least 3 temperatures in order to obtain a regression line at each end of the $De^- = f(1/T)$ plot. For this reason, Table 1 presents in **bold** the results obtained by means of the straight-lines with only **M = 2** representative points at the end of each De = f(1/T) plot, and using normal characters – the results given by the regression lines corresponding to M = 3 representative points at each end of the De=f(1/T) plot.

*Table 1*

**Study of a prediction criterion of the convergence behavior, starting from the zero-order approximations derived from the straight (regression, for M = 3) lines at the ends of the plot De = f(1/T), for different numbers M of temperatures considered at each plot end**

| STUDIED FEATURE | | Coordinates of the pixel | | | | |
|---|---|---|---|---|---|---|
| | | 29, 88 M=2 and M=3 | 61, 140 | | 31, 247 M = 2 | 41, 120 M=2 and M=3 |
| | | | M = 2 | M = 3 | | |
| Slopes ratio $s_{diff}/s_{dep}$ | | 1.6684 1.5776 | 2.165 | 1.834 | 1.97428 | 0.87969 1.0948 |
| Values of the zero-order approximations derived from the straight lines (regression lines for M = 3) at the end of the lnDe=f(1/T) plot | lnDiff$^{(0)}$ | 32.1206 | 32.13052 | 29.7451 | 31.0320 | 33.1328 |
| | lnDep$^{(0)}$ | 20.821 | 13.95848 | 17.00361 | 15.7293 | 51.2881 |
| | Eg$^{(0)}$(eV) | 1.0950 | 1.095144 | 1.00361 | 1.0668 | 1.12135 |
| | |Et-Ei|$^{(0)}$ (meV) | 108.801 | -41.74066! | 46.88855 | 6.9487 | 560.676 |
| Convergence behavior for the 0 order approximations obtained from | Regression lines at the ends of De = f(1/T) plot | Convergence | Instability | Convergence | Pseudo-convergence | Insta-bility Instability |
| | "central" zero-order approximations (see Table 2) | Convergence | CONVERGENCE | | Pseudo-convergence | Insta-bility |

One finds that: a) the above numerical scheme allows to predict the convergence behavior of the uniqueness parameters evaluation, b) a more detailed analysis of the stability field of the zero-order approximations is necessary in order to avoid the choice of such approximations outside this stability domain (see e.g. the case M=2 for the pixel 61,140 in the above table).

## 2.2. Criteria for the study of the local compatibility of theoretical models relative to the considered experimental data

A detailed study of the possibility to decide the compatibility/incompatibility of some theoretical models relative to the existing experimental data was achieved in the frame of [5]. This difficult problem is somewhat simplified if it is possible to admit a normal distribution of the individual values of the correlated parameters, in our case of dark current, $De^-$, and of their corresponding "inverse temperature" $\frac{1}{T}$.

In such a case, the confidence level $P_{conf.\tan g.}$ associated to the confidence ellipse (centered in the representative point of the most probable values of $De^-$ and $\frac{1}{kT}$), which is tangent to the theoretical plot $De^- = f\left(\frac{1}{kT}\right)$ can be used to estimate the error risk at the compatibility rejection:     $q = 1 - P_{conf.\tan g.}$     (12)

As the error risk, $q$, is less or larger than a certain threshold (usually between 0.1% and 2%), the compatibility hypothesis is rejected, or it has to be kept (accepted).

## 2.3. Choice of the zero-order approximations of the uniqueness parameters and some basic specific criteria for the pseudo-convergence identification

a) The values of the pre-exponential factor of the diffusion dark current
Given that the pre-exponential factors of the diffusion and depletion dark current, respectively, have very large values, we are obliged (by the computers numerical possibilities) to use the values of their logarithms: $\ln De^-_{0,diff}$ and $\ln De^-_{0,dep}$. According to reference [3b], we have chosen the zero-order approximation of the diffusion pre-exponential factor as: $\ln De^{(0)}_{0,diff} = 34.9$, but – according to our numerical results (see table **2**) - we can choose successfully these zero-order approximation with values between 32 and 53, which stand also inside the field of values with physical meaning.

b)  <u>The values of the pre-exponential factor of the depletion dark current</u>

According to reference [3b], we have chosen the zero-order approximation of the  depletion pre-exponential factor as: $\ln De^{(0)}_{0,diff} = 19.0$, but – according to our numerical results (see table **2**) - we can choose successfully these zero-order approximation with values between 18 and 30, which stand also for the limits of physical compatibility (results outside this interval representing almost sure an indicator of pseudo-convergence).

*Table 2*

**Synthesis of the obtained results concerning the: a) effective parameters of the semiconductor material (silicon with different impurities), b) the stability diameters around the representative point of the "central" zero-order approximations\*, starting from the temperature dependence of the dark current corresponding to the 20 selected pixels**

| Coordinates of the considered pixel | The effective value of the parameter (the "attractor coordinate") The extreme values of the stability diameter along this parameter\* | | | |
|---|---|---|---|---|
| | InDiff | InDep | Eg (eV)/ m $(m = 10 \times \frac{Eg0-EgAve}{EgSze-EgAve})$ | $\|Et-Ei\|$, meV |
| 41,120 | Instability | | | |
| 61,140 | $\frac{31.079047}{27 \ldots 54}$ | $\frac{17.524259}{15 \ldots 36}$ | $\frac{1.072556\ eV}{m = -6 \ldots +4}$ | $\frac{28.92\ meV}{2 \ldots 169\ meV}$ |
| 81,160 | $\frac{31.119436}{28 \ldots 56}$ | $\frac{16.276704}{16 \ldots 35}$ | $\frac{1.073807\ eV}{m = -8 \ldots +4}$ | $\frac{17.0\ meV}{3 \ldots 146\ meV}$ |
| 101,180 | $\frac{31.353146}{28 \ldots 55}$ | $\frac{15.706546}{15 \ldots 36}$ | $\frac{1.079606\ eV}{m = -8 \ldots +4}$ | $\frac{12.77\ meV}{3 \ldots 145\ meV}$ |
| 121,200 | $\frac{30.867372}{28 \ldots 55}$ | $\frac{15.611681}{17 \ldots 35}$ | $\frac{1.067257\ eV}{m = -10 \ldots +2}$ | $\frac{13.23\ meV}{0.9 \ldots 137\ meV}$ |
| 141,220 | $\frac{31.152358}{27 \ldots 54}$ | $\frac{15.684044}{14 \ldots 36}$ | $\frac{1.074538\ eV}{m = -10 \ldots +4}$ | $\frac{12.96\ meV}{3 \ldots 151\ meV}$ |
| 161,240 | $\frac{32.355596}{28 \ldots 55}$ | $\frac{19.409546}{17 \ldots 34}$ | $\frac{1.105744\ eV}{m = -6 \ldots +8}$ | $\frac{45.41\ meV}{1 \ldots 188\ meV}$ |
| 181,260 | $\frac{31.175348}{28 \ldots 54}$ | $\frac{15.508352}{16 \ldots 34}$ | $\frac{1.075505\ eV}{m = -10 \ldots +4}$ | $\frac{12.48\ meV}{1 \ldots 144\ meV}$ |
| 201,280 | $\frac{31.072543}{27 \ldots 55}$ | $\frac{16.904658}{15 \ldots 37}$ | $\frac{1.071989\ eV}{m = -6 \ldots +2}$ | $\frac{16.98\ meV}{2 \ldots 155\ meV}$ |
| 221,300 | $\frac{30.627558}{27 \ldots 54}$ | $\frac{16.588115}{15 \ldots 37}$ | $\frac{1.061095\ eV}{m = -10 \ldots +4}$ | $\frac{19.14\ meV}{2 \ldots 155\ meV}$ |
| 241,320 | $\frac{31.203713}{28 \ldots 54}$ | $\frac{15.338220}{17 \ldots 37}$ | $\frac{1.075681\ eV}{m = -10 \ldots +2}$ | $\frac{6.8\ meV}{0.64 \ldots 134 meV}$ |
| 261,340 | $\frac{31.768681}{28 \ldots 53}$ | $\frac{18.476570}{16 \ldots 34}$ | $\frac{1.090382\ eV}{m = -4 \ldots +8}$ | $\frac{30.22\ meV}{2 \ldots 149\ meV}$ |
| 281,360 | $\frac{31.117528}{27 \ldots 55}$ | $\frac{18.011161}{16 \ldots 35}$ | $\frac{1.073652\ eV}{m = -10 \ldots +4}$ | $\frac{27.51\ meV}{3 \ldots 164\ meV}$ |
| 301,380 | $\frac{30.193521}{27 \ldots 53}$ | $\frac{15.793308}{17 \ldots 33}$ | $\frac{1.048424\ eV}{m = -10 \ldots +2}$ | $\frac{11.58\ meV}{2 \ldots 137\ meV}$ |
| 321,400 | $\frac{31.241897}{28 \ldots 55}$ | $\frac{14.748118}{14 \ldots 34}$ | $\frac{1.076446\ eV}{m = -8 \ldots +6}$ | $\frac{18.21\ meV}{3 \ldots 160\ meV}$ |
| 341,420 | $\frac{33.174582}{28 \ldots 56}$ | $\frac{19.353229}{16 \ldots 33}$ | $\frac{1.126693\ eV}{m = -6 \ldots +4}$ | $\frac{30.77\ meV}{1 \ldots 181\ meV}$ |
| 31,247 | $\frac{35.635528}{27 \ldots 53}$ | $\frac{19.859227}{17 \ldots 32}$ | $\frac{1.190169\ eV}{m = -6 \ldots +6}$ | $\frac{10.3\ meV}{3 \ldots 180\ meV}$ |
| 29,88 | $\frac{31.261229}{28 \ldots 54}$ | $\frac{17.285039}{15 \ldots 35}$ | $\frac{1.077355\ eV}{m = -10 \ldots +4}$ | $\frac{24.15\ meV}{3 \ldots 155\ meV}$ |
| 188,471 | $\frac{31.097239}{28 \ldots 55}$ | $\frac{16.070513}{15 \ldots 32}$ | $\frac{1.071933\ eV}{m = -10 \ldots +6}$ | $\frac{22.05\ meV}{0.6 \ldots 151\ meV}$ |
| 161,289 | $\frac{31.838808}{32 \ldots 57}$ | $\frac{14.588399}{18 \ldots 30}$ | $\frac{1.092433\ eV}{m = -11 \ldots +10}$ | $\frac{28.36\ meV}{3 \ldots 130\ meV}$ |

* The values lnDiff = 34.9, lnDep = 19 [3b], $m = 0$, $|E_t - E_i| = 100$ meV were considered as "central". To determine the stability diameters, only one zero-order approximation is changed, the others remaining equal to the "central" values.

c)  <u>The criterion of the silicon energy gap $E_g$ estimation</u>

Because the usual values indicated by the specialty literature [6], [9], for the silicon energy gap for temperatures less than 300 K stand between 1.05 and 1.20 eV, the results outside this interval of the run programs represent almost sure an indicator of pseudo-convergence.

d) <u>The values of the difference of energies $|E_t - E_i|$ for the deep-level traps</u>

As it was shown above, the usual values of $|E_t - E_i|$ stand usually between 10 and 150 meV. Negative values of $|E_t - E_i|$ indicate obviously a pseudo-convergence of the run computer program.

**2.4. Study of the implications of the choice of the zero-order approximation of the value of the studied semiconductor effective energy gap**

Given being that the energy gap $E_g$ intervenes in the argument of both exponential functions, a first matter to be examined refers to the choice of its **zero-**order approximation.

Because: a) the first order approximation ($EgSze = 1.17\,eV$) indicated by Sze [7] for the silicon energy gap $E_g$ seems sometimes to be too large, we studied also the possibilities to choose this zero-order approximation by means of the:

b) modulus $EgLin$ of the slope of the straight-line joining the extreme points (for 222 K and 291 K, respectively) of the plot $\ln De^- = f\left(\dfrac{1}{kT}\right)$, with the meaning of an effective Arrhenius energy,

c) average of these zero-order approximations: $EgAve = \dfrac{1}{2}(EgSze + EgLin)$.

The implications of these 3 most important choices of the zero-order approximation of the energy gap of silicon on the evaluations of its uniqueness parameters are examined below.

**2.5. Study of the implications of the choice of the weights associated to the total dark current values**

a) Taking into account: (i) the huge differences between the very small values of dark current at low temperatures and the rather high ones at large temperatures, (ii) the necessity to describe accurately the whole studied

temperature range (222…291 K) of dark current, a first choice of the weights associated to the total dark current will correspond to the expression:

$$W_{ii}\left[De^-(T_i)\right] = \left[De^-(T_i)\right]^{-2} ,$$  (13)

so that the use of the classical gradient method will lead to a minimum value of the sum of squares of <u>relative</u> deviations of the calculated dark current in terms of their experimental values.

b) Assuming the (approximate) validity of a normal distribution of the experimental values of the studied parameters ($De^-$ and $\frac{1}{kT}$), the weights of the square deviations of the individual values relative to their most probable (true) ones will be  given by the inverses of their corresponding experimental variances, hence these inverses of variances will be kept as weights in the frame of the least-squares method:

$$W_{ii}\left[De^-(T_i)\right] = \frac{1}{V\left[De^-(T_i)\right]} .$$  (14)

The implications of these important choices of the: a) zero-order approximations of the uniqueness parameters, b) weights associated to the total dark current values, are  examined below.

### 3. Numerical Results

**3.1. Results concerning the compatibility of theoretical models relative to the considered experimental data**

a)      <u>Global compatibility: all dark current at different temperatures for a given pixel</u> (see also [5])

The accomplished study pointed out that – except pixel 41, 120 (with a global incompatibility relative to the assumed theoretical model) and pixel 31, 247, whose  experimental data lead to probably non-physical values of the uniqueness parameters (lnDiff, Eg, especially, and lnDep, |Et-Ei|, probably) - all other 18 pixels present experimental data in clear agreement with the considered theoretical model.

b)      **<u>Local compatibility of the dark current at a each temperature for different pixels</u>** (see also [5])

We have found a perfect local compatibility for temperatures T = 222, 232, 242,  252 and 291 K and rather frequent disagreements for the temperatures T = 262, 271 and 281 K. Taking into account that the standard deviations corresponding to these last 3 temperatures seem to be too optimistic, we studied the possibility to obtain a statistical agreement [according to relation (5)] for somehow larger values of the standard deviations for temperatures T = 262, 271

and 281 K. The accomplished study pointed out that 2 … 5 times larger values of the standard deviations for these last 3 temperatures re-establish the agreement between the corresponding experimental values and the studied theoretical model. That is why we consider that our study indicates that the standard deviations for these temperatures are in truth somewhat larger than the values indicated by Table 1 of work [1]).

### 3.2. Results about the (effective) values of the uniqueness parameters for different pixels

First of all, we have to underline that – due to the rather strong non-uniformity of the dark current corresponding to different pixels, it is expected to obtain rather different values of the uniqueness parameters of these pixels, these values corresponding to <u>effective parameters</u> **being due not only to** (the general use of) different experimental methods, but also to the non-uniformity of the studied physical systems (pixels).

The obtained effective values of the studied uniqueness parameters are located in the intervals (see also Table **2**):

(i) $\ln Diff$ - between 30 and 33.2 (the larger values as that: 35.6 for pixel 31, 247 being associated with non-physical values of other uniqueness parameters, e.g. |Et-Ei| ≈ 0.94 eV), (ii) $\ln Dep$ - between 15 and 19.5, (iii) |Et-Ei| between 13 and 91 meV, in agreement with the results obtained by means of other experimental methods in the frame of works [6] and [9], (iv) $Eg$ - between 1.06 and 1.13 eV.

### 3.3. Results concerning the numerical efficiency of different types of weights

As it was indicated above, we studied mainly the types of weights corresponding to relations (**13**) and (**14**). Unlike the behavior of the numerical fittings corresponding to relation (**13**) [incompatibility only for the pixel 41, 120 and probable pseudo-convergence for pixel 31, 247], we met considerably more bad fittings for the use of relation (**14**) [besides the pixels: (i) 41, 120 and (ii) 31, 247, there presented instabilities the experimental data corresponding to pixels: (iii) 101, 180, (iv) 121, 200, (v) 141, 220, (vi) 241, 320, (vii) 301, 380, (viii) 321, 400, (ix) 188, 471 and (x) 161, 289, i.e. the experimental data corresponding to a total number of 10 pixels (from the 20 studied ones) cannot be suitably processed by means of the weights described by relation (**14**)].

**It results that the use of relation (13), i.e. the minimization of the weighted sum of squares of <u>relative</u> deviations is clearly preferable.**

### 3.4. Results concerning the stability fields of the numerical processes of evaluation of the effective values of the uniqueness parameters

Starting from certain "central" values of the zero-order approximations of the specific uniqueness parameters: $\ln Diff^{(0)} = 34.9$, $\ln Dep^{(0)} = 19$ [3], |Et-Ei| = 0.1 eV and $m^{(0)} \cong 0$ ($m = 10 \times \dfrac{Eg0 - EgMed}{EgSze - EgMed}$), there were modified the values of only one uniqueness parameter (lnDiff, lnDep, $m$ or: |Et-Ei|, respectively). For each pixel, it was studied the behavior of the numerical process of evaluation of the uniqueness parameters:  the stability, and instability, respectively; the effective values of the uniqueness parameters, obtained as the corresponding coordinates of the attractor (in stability conditions, see Fig. 3); the appearance of the pseudo-convergence (when the attractor coordinates do not have a physical meaning); the existence (for weak attractors, see Table 3) of some significant oscillations in the frame of the numerical evaluation process (in stability conditions). The synthesis of the results obtained in the frame of this study allowed also to point out the stability fields diameters of the numerical evaluation processes corresponding to each uniqueness parameter [lnDiff, lnDep, $E_g$ (represented by $m$), and |Et-Ei|, in Table 2], for each of the studied pixels.
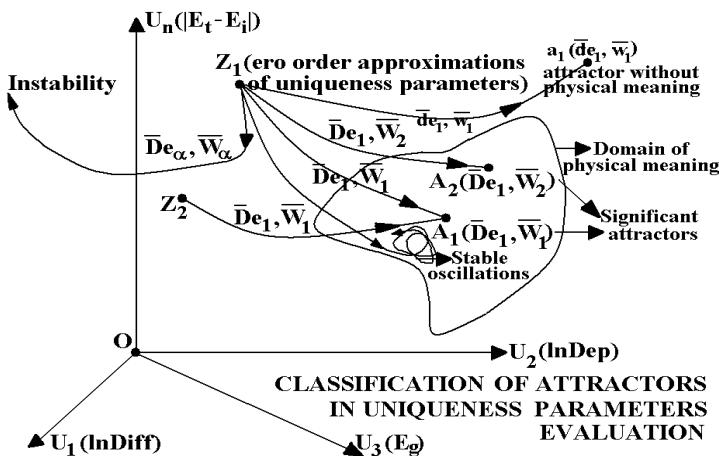


Fig. 3. Main types of evolution in the uniqueness parameters space of the representative point of evaluated values (example for the problem of temperature dependence of dark current in CCDs)

*Table 3*

**FINAL RESULTS (<u>concerning the values of uniqueness parameters**
**lnDiff, lnDep, E$_g$ and |E$_t$-E$_i$|</u>) OF THE GRADIENT METHOD USE for different pixels**
**and zero-order approximations of the uniqueness parameter lnDiff**

| Coordinates of the considered pixel | Zero order approximation of lnDiff | ln Diff | ln Dep | Eg(eV) | \|Et - Ei\| (meV) | Observations concerning the main features of the iterative process |
|---|---|---|---|---|---|---|
| 61, 140 | 34.9*** | 31.079047 | 17.524259 | 1.072556 | 28.92168 | *Very strong attractor:* |
| | 30 | 31.079047 | 17.524259 | 1.072556 | 28.92168 | *all 7 characteristic figures* |
| | 32 | 31.079047 | 17.524259 | 1.072556 | 28.92168 | *remaining invariable on the* |
| | 34 | 31.079047 | 17.524259 | 1.072556 | 28.92168 | *whole stability domain* |
| | 35 | 31.079047 | 17.524259 | 1.072556 | 28.92168 | |
| | 37 | 31.079047 | 17.524259 | 1.072556 | 28.92168 | |
| 121, 200 | 34.9*** | 30.867372 | 15.611681 | 1.067257 | 13.22839 | *Attractor of medium* |
| | 30 | 30.867402 | 15.613658 | 1.067257 | 13.24142 | *intensity, presenting* |
| | 32 | 30.867443 | 15.616538 | 1.067258 | 13.26039 | *also some medium* |
| | 34 | 30.867447 | 15.616764 | 1.067258 | 13.26188 | *amplitude oscillations* |
| | 35 | 30.867420 | 15.614914 | 1.067258 | 13.24970 | |
| | 37 | 30.867411 | 15.614337 | 1.067258 | 13.24590 | |
| 31, 247 | 34.9*** | 35.635528 | 19.859227 | 1.190169** | 10.30272 | *Pseudo-attractor* |
| | 30 | 35.635785 | 19.812839 | 1.190176** | 10.09618 | *(corresponding to a* |
| | 37 | 35.630835 | 21.082757 | 1.190045** | 15.24397 | *pseudo-convergence)* |
| 41, 120 | 34.9*** | | | | | |
| | 30 | *Instability, starting from the 3rd or 4th iteration* * | | | | |
| | 37 | | | | | |

\* The symbol "Instability starting from iteration **n**" indicates that – beginning from the succesive approximation (iteration) of the n-th order – the values of the studied parameters become larger than the divergence threshold admitted by the used computer. ** Values indicating the pseudo-convergence of the iterative numerical process, because they do not agree with the results of the experimental studies. *** The indicated value corresponds to the zero-order approximation chosen in the specialty literature [3b]

## 4. Conclusions

The use of the numerical analysis methods allowed:

1) to point out: (i) the global compatibility for the experimental results of 18 pixels from the 20 studied ones, (ii) the local compatibility for 5 from the 8 studied temperatures, as well as for the other 3 temperatures for somewhat larger values of the standard deviations of dark current, (iii) the agreement of the evaluated values of the distance |E$_t$-E$_i$| from the impurities (traps) energy level to that of the intrinsic Fermi level, with those obtained by different experimental methods [6], [9], [10], hence we consider that the accomplished numerical analysis confirms the compatibility of the quantum theoretical model Shockley-Read-Hall (SRH) [11], [12] with the experimental results referring to the temperature dependence of the dark current of the studied CCDs,

2) the emphasis (see table 2) of the basic types of results of the "fitting" processes (by means of the gradient method) of the parameters of Shockley-Read-Hall (SRH) nonlinear relations expressing the dark current in CCD: a) attractors,

whose components: (i) have a physical meaning, (ii) do not have a physical meaning (numerical processes of pseudo-convergence), b) oscillations inside the stability field, c) instabilities,

3) the evaluation of the effective values of the uniqueness parameters of the dark current of some Charge Coupled Devices (CCD): the pre-exponential factors of the diffusion and depletion  current, respectively, the forbidden band width $E_g$, and the difference $|E_t\text{-}E_i|$, as components of the positions of attractors resulted after the "fitting" processes of the parameters of the nonlinear Shockley-Read-Hall (SRH) relations,

4) the emphasis of the: a) considerably weaker effect of the temperature dependence of the forbidden band energy than that corresponding to impurities, b) principle possibility of numerical evaluation of the "polarization degree" $d$ of the cross-sections of capture corresponding to holes (σp) and electrons (σn), respectively:

$$d = \text{argtanh}[(\sigma p\text{-}\sigma n)/(\sigma p\text{+}\sigma n)],$$

5) the evaluation of the confidence domains of the pre-exponential factors: lnDiff = 31.2611 ± 0.5833 and lnDep = 16.6044 ± 1.42034. One finds so that while the relative square mean (standard) deviation of lnDiff (1.866%) stands in the limits of the experimental errors, that of lnDep (8.554%) is considerably larger (due to the specific contributions of traps).

The main goal of following studies will be to find if the present accuracy of the experimental determinations of the temperature dependence of the dark current in Charge Coupled Devices allows also: a) the effective evaluation of the "polarization degree" of the capture cross-sections for holes and electrons, respectively, b) the effective evaluation of both capture cross-sections $\sigma_n, \sigma_p$ corresponding to the free electrons and holes, respectively, c) the confirmation of the Meyer-Neldel correlations [3a] for the obtained uniqueness parameters.

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