STUDY OF THE NUMERICAL MODELING OF THE TEMPERATURE DEPENDENCE OF THE DARK CURRENT IN CHARGE COUPLED DEVICES (CCD)

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Abstract. *As it is well known, the classical works of the Dark Current Spectroscopy method allow - using some not too accurate theoretical relations, but huge numbers of dark current values for thousands of pixels - the evaluation of a reduced number of basic impurities parameters. Unlike these works, this paper tries to obtain – by means of some better approximations of the Shockley-Read-Hall (SRH) model - more information about the studied impurities, as well as the study of the compatibility of the used theoretical model SRH relative to the experimental data. In this manner, both the compatibility SRH model with the studied experimental data was checked up, as well as the values of some additional physical parameters of the impurified semiconductor (the logarithms of the pre-exponential factors lnDiff, lnDep, the effective value of the energy gap Eg) and of the separate capture cross-sections σ_n, σ_h of the free electrons, and holes, respectively, by the studied deep-level contaminants, were evaluated.*

Keywords: Dark Current Spectroscopy, Charge Coupled Devices chips, Dark Current, Shockley-Read-Hall model, Deep-level impurities, Capture Cross-Sections of Free electrons and holes

1. Introduction

As it is known (but not always checked up, by means of some specific compatibility criteria), the dark current in CCDs is described by the quantum theoretical model of Shockley-Read-Hall (SRH). It results that:

a) the dark current in CCDs in described by a huge number (unlimited, apparently) of (independent) uniqueness parameters, i.e. the studied CCDs are COMPLEX SYSTEMS,

b) this imposes the use of some APPROXIMATE RELATIONS (as the Arrhenius' one or the relations used by the classical works of the Dark Current Spectroscopy),

c) the values of the physical parameters obtained by means of these approximate relations depend on the specific features of each pixel, hence they are EFFECTIVE VALUES corresponding to some EFFECTIVE PARAMETERS, as: (i) the activation energy E_a from the Arrhenius' relation, (ii) the effective energy gap E_g intervening in the approximate relations, etc.

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d) in such conditions, it is possible to intervene some "hidden" relations, as the Meyer-Neldel one, but also (with different values of the correlation coefficient) some additional ones relative to certain parameters of the diffusion and depletion dark current, respectively, etc., the study of these (hidden) co-relations representing one of main tasks of this work.

In order to study the compatibility of the quantum SRH theoretical model (SRH) [1], [2] with the experimental data referring to the temperature dependence of the dark current in Charge Coupled Devices (CCD), starting from the experimental results reported by us in the frame of the works [3] - [5], we studied the evaluation of the corresponding dominant uniqueness parameters [6].

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 σ_n and holes σ_p , defined as: $d = \arg\tanh\left(\dfrac{\sigma_n - \sigma_p}{\sigma_n + \sigma_p}\right).$ (1)

The corresponding HSR expression of the total dark current was written as (see [5], [6]):

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

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

The accomplished study pointed out the compatibility of the HSR model with the indicated experimental data and allowed the evaluation of the chosen dominant uniqueness parameters, the obtained values being in agreement with the existing ones, obtained by means of different experimental methods [7], [8].

2. The Charge Coupled Devices (CCDs) as complex systems

In the frame of the study [5], we have found that even the classical (HSR) description of the CCDs semiconductor material requires a *huge (unlimited, practically) number of uniqueness parameters* (of usual symbols): D_n, x_c, A_{pix}, N_A, m_e, m_h, E_g, x_{dep}, n_i, σ_p, σ_n, V_{th}, N_t, n, p, $|E_t - E_i|$, etc, many of them [e.g. *n, p,* n_i , etc, 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].

Additionally, the electrons transitions from their "condensed" state in the valence band towards the free ("gaseous") state in the conduction band can be seen as a *phase transition*. For this reason, some descriptions of the Arrhenius' type of the temperature dependence of the currents in semiconductors are to be expected.

Finally, a CCD is composed by a *huge number* (of the magnitude order of 10^6) *of pixels*, with different and randomly distributed physical properties (see e.g. [9] and Fig. 1), *which imposes a statistical approach of their features*, hence all 3 basic characteristics of complex systems: huge number of uniqueness parameters, phase transitions and necessary statistical descriptions are reunited [10].
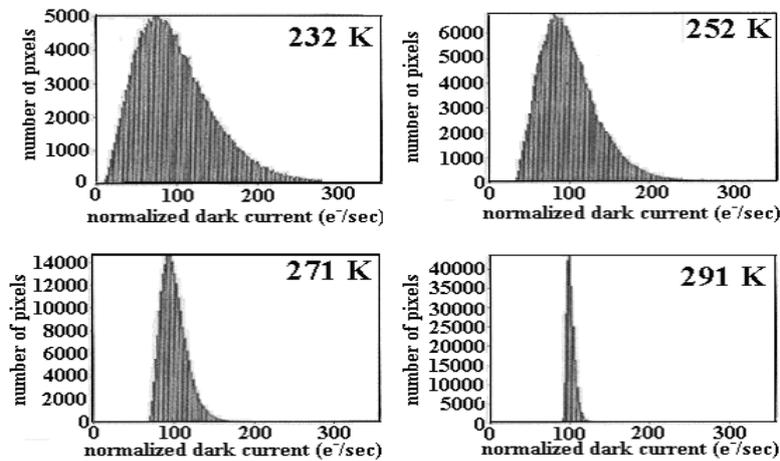
Fig. 1. Dark current normalized to 100 e⁻/s [9]

3. The dominant uniqueness parameters of the temperature dependence of electronic currents as effective parameters averaged over temperature

As it is well-known (see e.g. [11]), besides the directly measurable parameters, there is a large category of parameters whose values can be estimated starting from certain (assumed as valid) theoretical relations – the so-called *effective parameters*.

3.1. Thermionic Emission

Even in the rather simple case of the thermionic emission of metals (sometimes covered by a rather thin oxide layer), the description of the temperature dependence of the thermionic current requires the use of some effective parameters (averaged over temperatures) – the dominant ones being the pre-exponential factor (thermionic constant) A and the work function (extraction energy) φ defined by means of the Richardson-Dushman relation [12]:

$$j_s(T) = A \cdot T^2 \cdot \exp\left(-\frac{\varphi}{kT}\right) , \qquad (3)$$

where $j_s(T)$ is the saturation current density at temperature T and k is the Boltzmann's constant.

The classical work [13] presents (in the frame of table 4 of Chapter 3) a collection (starting from carbon: $A \approx 30$ A·cm^{-2}·K^{-2}, $\varphi \approx 4.34$ eV, up to uranium: ≈ 6 A·cm^{-2}·K^{-2}, 3.27 ± 0.05 eV) of 23 concomitantly estimated (by means of the least-squares fit) pairs of constants A and φ, for different metals. The correlation coefficient corresponding to these pairs is $r \approx 0.2275$ (and the square mean relative deviation corresponding to this regression line $s \approx 529.07\%$), hence the effective uniqueness parameters A and φ of the thermionic emission are independent.

3.2. Dark Current in Charge Coupled Devices

The dominant uniqueness parameters of the temperature dependence of the dark current in CCDs are obtained by means of some: a) partial, b) general (total) averages over temperatures. Unlike the state parameters $\ln Diff(T)$, $E_g(T)$, etc., which do not depend on the impurities features (concentrations, cross-sections, etc), the effective parameters $\ln Diff$, $E_{g,eff.}$, E_a, etc. depend on these features and on the considered pixel, implicitly.

    a) <u>The general (Arrhenius' type) CCDs dark current parameters averaged over temperatures</u>

Taking into account the above (negative) numerical result concerning the correlation of the pre-exponential factor A and of the corresponding work function (extraction energy) φ of the thermionic emission of metals, it results that almost sure the very strong (see e.g. [9] and Table 1 in following) Meyer-Neldel's type correlation [14] between the pre-exponential factor De_o and the Arrhenius activation energy E_a of the CCDs dark current [15]:

$$De(T) = De_o \exp\left(-\frac{E_a}{kT}\right) \qquad (4)$$

corresponds to a true physical relation between these effective parameters. Because this relation is not obvious, we will name in following such co-relations as « hidden » ones [16], they corresponding so to complex systems, with a huge number of (apparently) uniqueness parameters, sometimes in rather strong relations. We will underline here that our study [17] of several types of numerical simulations of different physical processes did not point out any type of numerical phenomenon (intervening in the least-squares procedures) which could be

misleading about the true or apparent (artifact) character of the studied physical relations, indicated by the statistical correlation coefficient.

    b) Partial (SRH type) CCDs dark current parameters averaged over temperatures

By means of a similar procedure, we can easily find that all 5 dominant uniqueness parameters intervening in the expression (2) of the dark current for the HSR model: $\ln De_{0,diff.}^- \equiv \ln Diff$, $\ln De_{0,dep.}^- \equiv \ln Dep$, $E_{g,eff.} \equiv E_g$, $E_t - E_i$ and d are *effective parameters*, whose values depend on the considered pixel, but are averaged over temperatures. Particularly, the HSR uniqueness parameter $E_{g,eff.} \equiv E_g$ has a net distinct physical meaning in comparison with any of the usual energy gap $E_g(T)$ parameters.

4. Study of the (co-)relations between the main uniqueness parameters of Dark Current in CCDs

The main studied uniqueness parameters were: a) the natural logarithms corresponding to the pre-exponential factors of the: (i) Arrhenius relation describing the temperature dependence of the dark current in CCDs, determined by means of the least-squares fit (regression line) method (denoted by ln*DArrh*), or as the intercept with the $\ln De$ axis of the straight-line joining the representative points (from the plane $\left\{ \ln De, \dfrac{1}{kT} \right\}$) corresponding to the extreme (222 and 291 K, respectively) temperatures (denoted as ln*Arrh*), (ii) diffusion (ln*Diff*) and depletion (ln*Dep*) terms, respectively, of the HSR expression (1) of the dark current in CCDs, b) the Arrhenius activation energy determined as the slope of the least-squares fit (regression) straight-line: $\ln De = f\left(\dfrac{1}{kT} \right)$ [*EaArrh*], or of the straight-line joining the representative points at the extreme temperatures [*EaLin*], c) the width of the forbidden band (energy gap) of the studied CCDs pixel (*Eg*), d) the modulus of the difference |*Et-Ei*| of energies corresponding to the capture center (trap) [*Et*] and to the intrinsic Fermi level (*Ei*), respectively, e) the *X*-coordinate of the studied pixel (*Xpixel*), f) the *Y*-coordinate of the studied pixel (*Ypixel*), g) the distance *R* of the considered pixel from the center of the studied CCD chip (*Rpixel*).

In order to find also : (i) the independent or co-related character of the considered uniqueness parameters, (ii) the influence of the theoretical description choice, we have evaluated (see Table 1) the corresponding correlation coefficients for the main pairs of the above indicated uniqueness parameters, corresponding to 3 simplifying hypotheses: a) null values of the modulus |*Et-Ei*| and of the capture

cross-sections polarization degree d, b) null value of d and considerably larger than 1 value of the ratio $\frac{|Et - Ei|}{kT}$, c) null value of d.

Table 1. Study of the main co-relations between the dominant uniqueness parameters of the dark current in CCDs

Correlation coefficient	Simplifying hypotheses		
	$Et = Ei$ **and** $d = 0$	$\|Et - Ei\| \gg kT$ **and** $d = 0$	$d = 0$
$\ln DArrh, EaArrh$	0.999918	0.9999656	0.9999022
$\ln Arrh, EaLin$	0.999949	0.9999591	0.9999350
$\ln DArrh, Eg$	0.8106086	0.2403149	0.1353221
$\ln Arrh, Eg$	0.7243172	0.2414372	0.2410846
$\ln Diff, Eg$	0.999945	0.999932	0.9997006
$\ln Dep, Eg$	0.737485	0.8810	0.574449
$\ln Diff, \|Et - Ei\|$	-	0.9518593	0.65158
$\ln Dep, \|Et - Ei\|$	-	0.9668592	0.747427
$Eg, \|Et - Ei\|$	-	0.9503131	0.6506456
$Eg, Xpixel$	- 0.43671	- 0.2813439	0.17089
$Eg, Ypixel$	- 0.13286	- 0.0976788	0.1269467
$Eg, Rpixel$	3.54×10^{-7}	1.947×10^{-7}	-5.367×10^{-7}

The analysis of the numerical results synthesized by Table 1 points out that: a) there is not any correlation between the energy width (gap) Eg of the forbidden band (as a representative parameter of the physical properties of the semiconductor material) and the co-ordinates OX, OY or the distance R to the center of the CCD chip, hence the semiconductor properties are randomly distributed for the pixels along these axes and around the center O,

      b) the very high values of the correlation coefficient corresponding to the pairs ($\ln DArrh, EaArrh$) and ($\ln Arrh, EaLin$) indicate that the genuine Meyer-Neldel relations [14]:

$$\ln De_O^- = \ln De_{oo}^- + \frac{E_a}{E_{MN}} \tag{5}$$

associated to the Arrhenius' relations [15]:

$$De^- = De_o^- \exp\left(-\frac{E_a}{kT}\right) \tag{6}$$

are fulfilled with high accuracy both for the equivalent Arrhenius' parameters ($\ln DArrh$, $EaArrh$) determined as the intercept and the slope of the least-squares fit (regression) line: $\ln De^- = f\left(\frac{1}{kT}\right)$ and as the intercept and slope ($\ln Arrh$, $EaLin$) of the straight-line joining the representative points corresponding to the extreme temperatures (222 and 291 K),

c) there is a strong asymmetry between the diffusion and depletion Meyer-Neldel's type relations for the semiconductor energy gap Eg: while the correlation ($\ln Diff$, Eg) is very strong, the correlation ($\ln Dep$, Eg) presents a medium or even a weak intensity,

d) the co-relations ($\ln DArrh$, Eg) and ($\ln Arrh$, Eg) keep (at limit) a medium intensity only for the obviously inaccurate assumption: $Et \neq Ei$, but they disappear totally for the calculations corresponding to non-null values of $|Et - Ei|$,

e) the modulus $|Et - Ei|$ of the energies corresponding to the capture centers (traps) Et and to the intrinsic Fermi level Ei, respectively, presents at least weak co-relations with all main uniqueness parameters: $\ln Diff$, $\ln Dep$ and Eg of the dark current in CCDs.

5. Interpretation possibilities of dark current non-uniformity in CCD chips by means of the « hidden » (of the Meyer-Neldel's type) correlations

5.1. Meyer-Neldel's type relations referring to the diffusion dark current

Taking into account that the correlation ($\ln Diff$, Eg) is much stronger than the ($\ln Diff$, $|Et - Ei|$) one [r($\ln Diff$, Eg) $\approx$ 0.999706, while r($\ln Diff$, $|Et - Ei|$) is only 0.65158], we will neglect the influence of $|Et - Ei|$ values on the diffusion dark current non-uniformity.

The regression line corresponding to the strong ($\ln Diff$, Eg) correlation is described by the equation: $\ln Diff = i + s \cdot E_g$, where the intercept (coordinate of the crossing point with the $\ln Diff$ axis) is $i \approx -10.01989$ and the slope $s \approx 38.3229 \text{eV}^{-1}$, its accuracy being also very high (standard relative deviation of only 0.21048%).

According to relation (2), the temperature dependence of the diffusion dark current can be written as:

$$De_{diff}^- = \exp\left[i + E_g\left(s - \frac{1}{kT}\right)\right] \cdot T^3 = \exp\left[i + \frac{E_g}{k}\left(\frac{1}{T_o} - \frac{1}{T}\right)\right] \cdot T^3, \tag{7}$$

its characteristic temperature being: $T_o = \dfrac{1}{k \cdot s} \approx 302.8086$ K.

Because the characteristic temperature T_o is rather near to the studied temperatures (222 … 291 K) [hence the differences $\dfrac{1}{T_o} - \dfrac{1}{T}$ are rather small] and the correlation coefficient r($\ln Diff, |Et - Ei|$) is very high, the non-uniformity of the dark current at high temperatures (where the diffusion dark current prevails) is reduced (see Figs. 1).

5.2. "Hidden" (of Meyer-Neldel's type) co-relations referring to the depletion dark current

Taking into account the rather near values of the correlation coefficients r($\ln Dep, Eg$) ≈ 0.57449 and r($\ln Dep, |Et - Ei|$) ≈ 0.747427, we studied the double linear regression: $\ln Dep = f(Eg, |Et - Ei|) = i' + s_1 \cdot Eg + s_2 \cdot |Et - Ei|$,   (8)

determining its basic parameters:

  a) correlation coefficient r($\ln Dep; Eg, |Et - Ei|$) ≈ 0.756385,

  b) standard relative deviation $\approx 6.01144\%$,

  c) coordinate of the crossing point with the lnDep axis: $i' \approx 0.45434$,

  d) slope relative to E_g: $s_1 \approx 13.04339$ eV^{-1},

  e) slope relative to $|E_t-E_i|$: $s_2 \approx 49.390135$ eV^{-1}.

Starting from relation (2), one finds that the expression of the temperature dependence of the depletion dark current is:

$$\overline{De}_{dep} = \exp\left[i' + E_g\left(s_1 - \frac{1}{2kT} \right) + |E_t - E_i| \cdot s_2 \right] \cdot \frac{T^{3/2}}{\cosh\left(\dfrac{|E_t - E_i|}{kT} \right)} \ . \qquad (9)$$

In order to define also a characteristic temperature of the ($\ln Dep, |Et - Ei|$) correlation, we will consider the particular case: $x = \dfrac{|E_t - E_i|}{kT} \gg 1$, when the hyperbolic cosine can be approximated as: $\cosh x \cong \dfrac{1}{2} \cdot e^x$. In this approximation, the above relation can be written as:

$$\overline{De}_{dep} \cong 2\exp\left[i' + \frac{E_g}{2k}\left(\frac{1}{T_1} - \frac{1}{T} \right) + \frac{|E_t - E_i|}{k}\left(\frac{1}{T_2} - \frac{1}{T} \right) \right] \cdot T^{3/2} \ , \qquad (10)$$

where the characteristic temperatures corresponding to the ($\ln Dep$, Eg) and to the ($\ln Dep$, $|Et - Ei|$) correlation, respectively, are:

$$T_1 = \frac{1}{2k \cdot s_1} \cong 444.8426 \text{ K}, \qquad T_2 = \frac{1}{k \cdot s_2} \cong 234.956 \text{ K}.$$

Given being that:

a) while the characteristic temperature of the ($\ln Dep$, $|Et - Ei|$) correlation is located inside the studied temperature interval (222 … 291 K), that corresponding to the ($\ln Dep$, Eg) correlation is (444.8426 K) rather distant relative to this interval, b) the correlation coefficient r($\ln Dep$, $|Et - Ei|$) ≈ 0.747427 is considerably larger that of the ($\ln Dep$, Eg) correlation: r($\ln Dep$, Eg) ≈ 0.574449, it results that the large spreading of the depletion dark current (which prevails at low temperatures, see Figs. 1) is due mainly to the weak ($\ln Dep$, Eg) correlation (see also [18]).

5.3. Implications of the asymmetry of the diffusion and depletion Meyer-Neldel's type relations on the non-uniformity of dark currents

Assuming that the pairs of individual values ($\ln Dep$, Eg), ($\ln Dep$, $|Et - Ei|$), ($\ln Diff$, Eg), etc. are normally distributed around their average values <lnDep>, <Eg>, etc. and denoting by $X = Eg - <Eg>$, $Y = \ln Dep - <\ln Dep>$, etc. the corresponding deviations, the equation of the confidence ellipses is:

$$\frac{X^2}{\sigma^2(X)} + \frac{Y^2}{\sigma^2(Y)} - 2r \frac{X}{\sigma(X)} \cdot \frac{Y}{\sigma(Y)} = p \ , \tag{11}$$

where $\sigma(X), \sigma(Y)$ and r are the corresponding standard deviations and the correlation coefficient, while p is a parameter related to the confidence level associated to the considered confidence ellipse (11):

$$p = -2\left(1 - r^2\right) \cdot \ln(1 - L) . \tag{12}$$

Scaling the physical units to have equal standard (square mean) deviations: $\sigma(X), \sigma(Y)$, it results (see e.g. [11], p. 40) that the ratio of the semi-minor axis b to the semi-major axis a of the confidence ellipse relative to its symmetry axes (see also Fig. 2) is:

$$\frac{b}{a} = \sqrt{\frac{1 - r}{1 + r}} \ . \tag{13}$$

One finds so that for the ($\ln Dep$, Eg) and ($\ln Diff$, Eg) co-relations, the values of this ratio are:

$$\left(\frac{b}{a}\right)_{\ln Dep, Eg} \cong 0.51989 \quad \text{and} \quad \left(\frac{b}{a}\right)_{\ln Diff, Eg} \cong 0.012236 .$$

These values explain also the considerably higher non-uniformity of the dark current at low temperatures (when the depletion dark current prevails) than at high temperatures (in conditions of diffusion dark current prevalence).
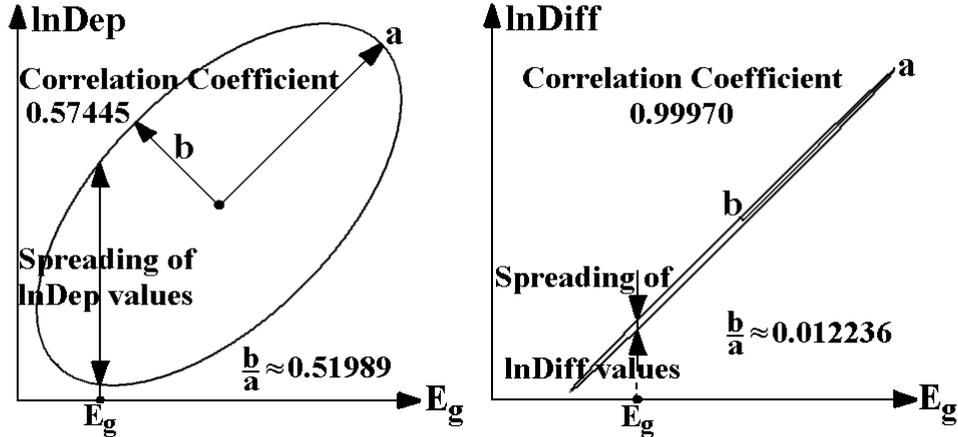
Fig. 2. The confidence ellipses associated to assumed normally distributed pairs of individual values ($\ln Dep$, Eg) and ($\ln Diff$, Eg), for the $\sigma(X) = \sigma(Y)$ scaling.

6. Conclusions

The accomplished study of the possible co-relations between the basic uniqueness parameters ($\ln De^{-}_{0,diff} \equiv \ln Diff$, $\ln De^{-}_{0,dep} \equiv \ln Dep$, E_g and $|E_t\text{-}E_i|$) of the temperature dependence of the dark current in CCDs pointed out the presence of some strong or at least weak co-relations relating the (natural logarithms of) pre-exponential factors $\ln Diff$ and $\ln Dep$ both with the energy gap Eg and with the modulus of the energy difference corresponding to the capture traps Et and to the intrinsic Fermi level E_i.

This study pointed out also that the experimental finding referring to the considerably larger non-uniformity of the dark current at low temperatures than at higher ones is due both to: a) the considerably stronger Meyer-Neldel type correlation ($\ln Diff$, Eg) than the ($\ln Dep$, Eg) one [see figs. 2], b) the location of the characteristic temperatures of the ($\ln Diff$, Eg) and ($\ln Dep$, $|Et - Ei|$) co-relations very near or even inside the studied temperatures interval (which minimizes also the corresponding spreading of the dark current values), while the characteristic temperature of the ($\ln Dep$, Eg) correlation is located considerably outside the studied temperatures interval, leading also to a considerably larger dark current non-uniformity at low temperatures (when the depletion dark current is prevalent).

The obtained results underline so the theoretical and practical importance of the study of the "hidden" co-relations between the physical parameters of complex materials, being of particular interest for the technical applications of CCDs (see [19], [20]).

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