NEW MEYER-NELDEL RELATIONS FOR THE DEPLETION AND DIFFUSION DARK CURRENTS IN SOME CCDs

E. BODEGOM, R. WIDENHORN*, D. A. IORDACHE**

* Department of Physics, Portland State University, Portland, Oregon, USA, OR97207
E-mail: Bodegom@pdx.edu
** Physics Department, University "Politehnica", Splaiul Independenţei 313, Bucharest 77206,Romania
E-mail address: daniordache2003@yahoo.com

Abstract–The temperature dependence of the dark currents in some Charged - Coupled Devices (CCDs) was studied. The obtained results point out: a) the compatibility of the theoretical description of these dark currents by means of depletion and diffusion processes, resp. relative to the experimental data, b) the possibility to evaluate – for each pixel – the difference of energies corresponding to the generation-recombination centers and to the intrinsic Fermi *level, resp., c) some new Meyer - Neldel relations between the exponential pre-factors corresponding to the depletion and diffusion currents, resp. and the energy gap E_g of studied semiconductor materials.*

Keywords:* *Depletion and Diffusion Dark Currents, Charged-Coupled Devices, Meyer-Neldel relations

1. INTRODUCTION

The dark currents corresponding to backside-illuminated Charged-Coupled Devices (CCDs) housed in SpectroVideo camera (model SV512 V1, manufactured by Pixelvision, Inc.) were determined [1], [2]. The CCD chip (12.3 mm × 12.3 mm) is composed of an array of metal oxide semiconductor capacitors (512 × 512 pixels, manufactured by SITE Inc., the individual pixel size being 24 μm × 24 μm). An external field collected the thermally excited electrons separately for each pixel. When the chip is not exposed to light, these electrons cause the so-called *dark count (current)*. Due to impurities (which enhance significantly the dark currents and are also responsible for other unwanted effects, as the residual images in astronomy [3], [4]), the dark count is not uniform for all pixels.

As many thermally activated processes, the dark currents obey the exponential Arrhenius law:

$$De^- = De_0^- \exp(-\Delta E / kT) \ , \qquad (1)$$

where De^- is the dark current in e^-/s (or counts/s) and ΔE is the activation energy. As a consequence, the average values of the dark currents increase exponentially towards the higher temperatures, being for 20 randomly chosen pixels: approx. 0.00978 counts/s at T = 222 K, 0.0387 counts/s (232 K), 0.13602 counts/s (242 K), 0.58805 counts/s (252 K), 2.39416 counts/s (262 K), 10.217 counts/s (271 K), 46.6347 counts/s (281 K) and 223.4327 counts/s at 291 K.

In order to minimize the errors, the dark counts were calculated as the average of the values corresponding to 50 pictures taken for each of the exposure times: 3, 5, 10, 20, 50, and 100 s, 20 images each for 250 and 500 s and finally 10 pictures at 1000 s. The relative standard (square mean) deviations corresponding to the *dispersion* of the individual values of the dark currents corresponding to each temperature were: approx. 35.85% at T=222 K, 9.45% (232 K), 3.53% (242 K), 1.03% (252 K), 0.486% (262 K), 0.233% (271 K), 0.233% (281 K) and 0.297% (291 K). The standard error corresponding to our temperature determinations was approximately 1 K.

2. METHODS

Because the dark current in a CCD is an important source of noise, it has been studied in detail. It was found that for a CCD used in multipinned phase (MPP) mode the *Si-SiO*$_2$ interface is inverted with a high hole carrier concentration and the surface dark current generated at this interface is almost completely suppressed. That is why the main sources of dark current remaining in our case are: (i) the depletion or bulk current generated in the depletion region, (ii) the diffusion dark current generated in the field-free region. The description of these currents is very similar to the description of dark currents in semiconductor diodes [5].

a) Depletion Dark Current

In the depletion region, the electric field sweeps holes to the *p*-region and electrons to the *n*-region. Consequently, there is a region depleted of carriers, where the electron (n) and hole (p) concentrations are much less than the intrinsic (n_i) carrier concentration: $n, p << n_i$. The expression of the recombination and generation rates U of carriers through intermediate centers (impurities or defects) given by Hall, Shockley and Read [6]-[8] becomes:

$$U_{dep} = \frac{A \cdot n_i}{\cosh\left[\dfrac{E_i - E_t}{kT}\right] + \dfrac{\sigma_p - \sigma_n}{\sigma_p + \sigma_n}\sinh\left[\dfrac{E_i - E_t}{kT}\right]} \ , \qquad (2)$$

where:

$$A = \frac{v_{th} N_t \sigma_p \sigma_n}{\sigma_p + \sigma_n} \ , \qquad (3)$$

E_i is the intrinsic Fermi level, N_t – the concentration of bulk generation-recombination centers at the energy level E_t, v_{th} is the thermal velocity, σ_p and σ_n are the capture cross-sections for holes and electrons, respectively, and the intrinsic carrier concentration n_i is given by the relation:

0-7803-8499-7/04/$20.00 © 2004 IEEE

$$n_i = \sqrt{N_v N_c}\exp\left(-\frac{E_g}{2kT}\right) = c_n T^{3/2}\exp\left(-\frac{E_g}{2kT}\right), \qquad (4)$$

where N_v and N_c are the effective density of states for the valence and conduction band, respectively.

Taking into account that the dark current density per unit surface generated in the depletion region is:

$$I_{dep} = q x_{dep} U_{dep}\ , \qquad (5)$$

it results that the depletion dark current in e^-/s (or *counts/s*) per pixel is:

$$De^-_{dep} = x_{dep} A_{pix} U_{dep}\ , \qquad (6)$$

where q is the electron charge, x_{dep} the size of the depletion region and A_{pix} is the area of the pixel.

If the capture cross-sections for holes and electrons are approximately equal: $\sigma_p \approx \sigma_n$, the relations (2), (4) and (6) lead to:

$$De^-_{dep} = De_{0,dep} T^{3/2}\frac{\exp\left(-\dfrac{E_g}{2kT}\right)}{\cosh\left[\dfrac{E_i - E_t}{kT}\right]}\ , \qquad (7)$$

where the pre-factor corresponding to the depletion dark current is:

$$De_{0,dep} = A\,.c_n x_{dep} A_{pix}\ . \qquad (8)$$

Finally, if the bulk generation-recombination centers are located close to the mid-gap: $E_t \approx E_i$, the expression (7) becomes:

$$De^-_{dep} = De_{0,dep} T^{3/2}\exp\left(-\frac{E_g}{kT}\right). \qquad (9)$$

b) Diffusion Dark Current

Assuming that the size x_{ff} of the CCD which remains field-free is smaller than the diffusion length L_n, the carrier concentration in this region is:

$$n_p = n_{p0}\frac{x}{x_{ff}}\ , \qquad (10)$$

where the equilibrium minority carrier concentration is:

$$n_{p0} = \frac{n_i^2}{N_A}\ , \qquad (11)$$

N_A being the concentration of the p-doped material (in our case – boron). It results that the diffusion current is:

$$I_{diff} = qD_n\frac{dn_p}{dx} = \frac{qD_n n_i^2}{x_{ff} N_A}\ , \qquad (12)$$

where D_n is the diffusivity of electrons, while the diffusion dark current in e^-/s (or *counts/s*) per pixel is:

$$De^-_{diff} = \frac{A_{pix}}{q} I_{diff} = De_{0,diff} T^3\exp\left(-\frac{E_g}{kT}\right), \qquad (13)$$

and the pre-factor corresponding to the diffusion dark current is:

$$De_{0,diff} = \frac{A_{pix} D_n \cdot c_n^2}{x_{ff} N_A}\ . \qquad (14)$$

3. MAIN FEATURES OF THE USED (COMPUTER) ALGORITHMS

a) Gradient Method

In order to search the specific values (to each pixel) of the material parameters p_j (as E_g, $De_{0,dep}$, $De_{0,diff}$, $|E_t - E_i|$, etc), we used the classical version [9], [10] of the (deterministic) gradient method, improved by the introduction [11] of the damping factors λ (≤ 1), used to avoid the divergence of the iterative procedure:

$$\overline{C}^{(I)} = -\left(\overline{\overline{J}}^{(I)^T}\,\overline{\overline{W}}\cdot\overline{\overline{J}}^{(I)}\right)^{-1}\cdot\overline{\overline{J}}^{(I)^T}\,\overline{\overline{W}}\cdot\overline{D}^{(I)}\ , \qquad (15)$$

where $\overline{C}^{(I)}$ is the vector of material parameters corrections in the iteration I, $\overline{D}^{(I)} = \bar{t}^{(I)}_{calc} - \bar{t}_{\exp}$ is the vector of the deviations of calculated values of the test parameters [the total values of dark currents at different temperatures $De^-(T) = De^-_{dep}(T) + De^-_{diff}(T)$] relative to the experimental values $\bar{t}_{\exp}$, $\overline{\overline{J}}$ is the jacobian matrix, whose elements are defined as:

$$J^{(I)}_{ij} = \frac{\partial t^{(I)}_{calc.}}{\partial p_j}\ , \qquad (15)$$

and $\overline{\overline{W}}$ is the matrix of weights, chosen usually as:

$$W_{ij} = \frac{1}{t^2_{\exp}}\delta_{ij}\ , \qquad (16)$$

where δ_{ij} is the Kronecker's symbol.

Taking into account the empirical expression of the band gap of *Si* [12]:

$$E_g(T) = 1.17\ eV - \frac{4.73\times10^{-4}T^2}{T+636}\ , \qquad (17)$$

the zero-order approximation of E_g was chosen usually as the average of Sze's threshold value E_{g0}= 1.17 eV and the value obtained for the activation energy:

$$De^- = De^-_{dep} + De^-_{diff} = De_0\exp\left(-\frac{E_a}{kT}\right), \qquad (18)$$

starting from the experimental dark currents corresponding to the extreme studied temperatures (222 and 291 K).

We used also – as zero-order approximations of the pre-factors – the values: $De_{0,dep}$ = exp(19) $e^-/K^{3/2}$ and $De_{0,diff}$ = =exp(34.9) e^-/K^3 indicated by work [2], p.29.

b) Local Compatibility Tests

Taking into account that our work is intended to the study of the compatibility of the above theoretical model with the obtained experimental data, as well as the specific errors affecting these experimental data, we are interested to study the compatibility of the theoretical model best-fitting (given by the gradient method for each pixel) with the experimental results corresponding to each temperature. Starting from the confidence domain (ellipse) associated to the normally distributed values x_i , y_i of the parameters X, Y [13]-[15], corresponding to the state i defined by the most probable values x_{imp} , y_{imp}:

$$\left[\frac{x_i - x_{imp}}{s(x_i)}\right]^2 + \left[\frac{y_i - y_{imp}}{s(y_i)}\right]^2 - 2r_i\frac{x_i - x_{imp}}{s(x_i)}\frac{y_i - y_{imp}}{s(y_i)} = f(L_i)\ , \qquad (19)$$

where $s(x_i)$, $s(y_i)$ are the square mean deviations (errors) of the individual values x_i, y_i corresponding to the state i, r_i is the correlation coefficient of these deviations, and:

$$f(L_i) = -2\left(1 - r_i^2\right)\cdot\ln L_i\ , \qquad (20)$$

L_i being the confidence level associated to the confidence ellipse (19).

Let $f(L_{ti})$ be the value of the expression (19) corresponding to the confidence ellipse E_{ti} tangent to the plot $Y = f(X)$ of the studied theoretical relation. Taking into account that the parameters:

$$q_i = 1 - \exp\left[-\frac{f_2(L_{ti})}{2\left(1 - r_i^2\right)}\right] \qquad (21)$$

corresponds to the probability to find the representative point (x_i, y_i) outside the confidence ellipse E_{ti}, it results that the parameters q_i evaluate the error risk at the rejection of the compatibility of the studied theoretical relation $Y = f(X)$ relative to the pair of individual values (x_{imp}, y_{imp}) [16].

As the error risk $q_i<0.001$ or $q_i>0.02$, the statistical hypothesis concerning the compatibility of the theoretical relation $Y = f(X)$ relative to the pair of individual values (x_{imp}, y_{imp}) is rejected or it is accepted, respectively.

c) Final (physical) tests

According to the empirical expression (17) of Sze [12], the energy gap E_g corresponding to *Si* would be approx. 1.1474 eV at 200 K and 1.1245 eV at 300 K. Because the E_g values determined from the dark currents correspond to an effective parameter (whose values depend somewhat on the used experimental method, as well as on the chosen temperature interval), it is expected to obtain E_g values between 1 eV and 1.2 eV.

Taking into account that both the depletion and the diffusion dark currents are thermally activated processes, it is expected that – if their contributions to the total dark current were correctly separated by means of the used computer algorithm – their pre-factors and activation energies (e.g. E_g) will fulfill some correlations of the Meyer-Neldel [17] type, perhaps even better than the Arrhenius' type relation corresponding to the total dark current.

4. RESULTS

a) Compatibility of the Theoretical Model relative to the Experimental Results

We studied firstly the compatibility of the theoretical model expressed by the relations (9) and (13) relative to the experimental data corresponding to 20 somewhat randomly chosen pixels, at different temperatures. Taking into account that the relative errors corresponding to the lower temperatures are somewhat larger (see Section 1), we accomplished the fitting of the material parameters for the highest 6 temperatures ($T \geq 242$ K), but we tested finally the compatibility of the obtained theoretical descriptions for the lowest considered temperatures (222 and 232 K).

Assuming that the standard errors affecting the measured dark currents are approximately those corresponding to the *dispersion* of the individual values (whose average relative errors were indicated in Section 1), the percentages of the measured dark currents compatible with the theoretical model are: 100% compatibility of the experimental data corresponding to the temperatures 232 and 242 K, resp., 90% compatibility (2 incompatibility cases from the 20 studied pixels) for 222 K, 65% compatibility for 291 K, 60% compatibility cases for 252 K and only 25% compatibility cases for the 262 K dark currents and 5% compatibility for 271 and 281 K, resp. One finds also that all measured dark currents are compatible with the studied theoretical model if the true standard errors corresponding to the "higher" temperatures are somewhat larger: approx. 1.12% at 252 K, 0.71% at 262 and 271 K, resp., 0.81% at 281 K, and 0.37% at 291 K, instead of the corresponding dispersion errors: 1.03% (252 K), 0.486% (262 K), 0.233% (271 and 281 K), 0.297% (291 K).

The analysis of these findings points out: (i) the compatibility of the theoretical model expressed by relations (9) and (13) with the obtained experimental results, (ii) the possibility of such theoretical descriptions of the temperature dependence of the dark currents with average errors between 0.96% and 3.79% (for the temperature domain 242...291 K) and between 3.29% and 18.27% (for the entire studied domain 222...291 K), depending on the studied pixel, (iii) the true standard errors are somewhat larger than the dispersion ones, for the temperatures between 262 and 281 K, especially.

b) The evaluation of the difference of energies corresponding to the bulk generation-recombination centers and to the intrinsic Fermi level, resp.

We studied also the compatibility of the theoretical model expressed by the relations (7) and (13) relative to the experimental data.

We have found the compatibility of 90% of the experimental data sets (for 18 pixels from the 20 studied ones) with this model. This results indicates that generally the capture cross-sections for holes and electrons are approximately equal: $\sigma_p \approx \sigma_n$. The remaining 10% cases require the more sophisticated description given by the relation (2), corresponding to rather different values of the capture cross-sections σ_p , σ_n . The obtained values of the $|E_t - E_i|$ differences are between 15.5 and 91 meV, i.e. of the magnitude order of the thermal energy (kT).

The accuracy of the description of $De^- = f(T)$ dependencies ensured by the relations (7) and (13) is considerably better (relative errors between 0.7% and 3.16%, with an average of 2.36%),than that given by relations (9) and (13) (relative errors between 0.96% and 3.79%, with an average of 2.72%). The square mean deviation [relative to the value $E_g = 1.135$ eV given by the Sze's empirical relation (17) for the average temperature $T = 256.5$ K corresponding to the studied temperature domain] of the evaluated (for the 18 compatibility cases) E_g values by means of the relations (7) and (13): 58.5 meV is also considerably better than the corresponding deviation (93.42 meV) associated to relations (9) and (13).

c) Newly identified Meyer-Neldel correlations

The work [1] has pointed out the outstanding fulfillment of the Meyer-Neldel rule by the exponential pre-factor De_0 and the activation energy ΔE corresponding to the temperature dependence (1) of the dark currents. For the 20 studied pixels, we obtained the remarkably high value of the correlation coefficient associated to this Meyer-Neldel relation: $r\left(\ln De_0^-, \Delta E\right) \cong 0.999918$.

Taking into account that the depletion and diffusion processes are also thermally excited phenomena, we studied the correlation coefficients corresponding – for different theoretical models – to the pairs ($\ln De_{0,dep}$, E_g) and ($\ln De_{0,diff}$, E_g), resp. The obtained results are indicated in Table 1.

Table 1. *Correlation Coefficients of Some New Meyer-Neldel Relations*

Theoretical Model	Correlation Coefficients	
	ln $De_{0,dep}$, E_g	ln $De_{0,diff}$, E_g
Relations (9) and (13)	0.737485	0.999945
Relations (7) and (13)	0.882099	0.999931
Parabolic $E_g(T)$ dependence	0.9985505	0.9992202

One finds that the pre-factors and the band gap energy E_g values fulfill some specific Meyer-Neldel relations, whose correlation coefficients are sometimes (for the diffusion contribution, whose values are considerably more accurate evaluated by the used theoretical models) even higher than that of the original (Arrhenius) Meyer-Neldel relation. The improvement of the theoretical model (taking into account the effect of the different energies of the generation-recombination centers and of the intrinsic Fermi level, resp., the temperature dependence of E_g, etc) leads to an increase of the correlation coefficients, even if some of the corresponding hypotheses (e.g. of the parabolic $E_g(T)$ dependence) were not quantitatively compatible with the studied experimental data.

5. CONCLUSIONS

The accomplished numerical analysis of the experimental data corresponding to 20 somewhat randomly chosen pixels of a Charge-Coupled Device pointed out:

a) the compatibility of the description of the temperature dependence of the dark currents in the studied CCDs by means of the classical theory of depletion and diffusion processes, relative to the obtained experimental data,

b) the existence of some systematic errors concerning the measured dark currents, additional to those evaluated starting from the dispersion of the individual values,

c) the possibility to evaluate for each pixel the difference of energies corresponding to the generation-recombination centers and to the intrinsic Fermi level, resp.

d) some new Meyer-Neldel relations between the exponential pre-factors corresponding to the depletion and diffusion currents, resp. and the band gap energy E_g of the studied semiconductor materials.

The further studies will be intended to the evaluation of the "polarization" factor $\dfrac{\sigma_p - \sigma_n}{\sigma_p + \sigma_n}$ corresponding to the capture cross-sections for holes and electrons, resp., as well as to the study of some empirical relations (as the Sze's one [12]) describing the temperature dependence of the band gap energy E_g in the studied semiconductor materials.

REFERENCES

[1] R. Widenhorn, L. Münderman, A. Rest, E. Bodegom, *J. Appl. Phys.*, vol. 89, no.12, pp. 8179, 2001.

[2] R. Widenhorn, E. Bodegom, "Interpreting Fitting Parameters", in *Proceedings of the 2nd Colloquium "Mathematics in Engineering and Numerical Physics"* (MENP-2), Bucharest, part 2, pp. 26-30, 2002.

[3] A. Rest, L. Münderman, R. Widenhorn, T. McGlinn, E. Bodegom, "Residual Images in Charge-Coupled Devices" (to be published).

[4] J.R. Janesick, T. Elliot, S. Collins, M. Blouke, J. Freeman, *Opt. Eng.*, vol. 26, 1987.

[5] A.S. Grove, *Physics and Technology of Semiconductor Devices,* John Wiley & Sons, New York, 1967.

[6] C.T. Sah, R.N. Noyce, and W. Shockley, *Proc. IRE,* vol. 45, pp. 1228, 1957.

[7] R.N. Hall, *Phys. Rev.,* vol. 87, pp. 387, 1952.

[8] W. Shockley, W.T. Read, *Phys. Rev.,* vo. 87, pp. 835, 1952.

[9] [9] K. Levenberg, "A method for the solution of certain non-linear problems in least-squares", *Quart. Appl. Math.,* vol. 2, pp. 164-168, 1944.

[10] D.W. Marquardt, "An algorithm for least-squares estimation of non-linear parameters", *Journal of Society Industr. Appl. Math.,* vol. 11, pp. 431-441, 1963.

[11] Z. Mei, J.W. Morris jr., *J. Nucl. Instr. Methods in Phys. Res.,* vol. 6, pp. 371, 1990.

[12] S.M. Sze, *Physics of Semiconductor Devices,* 2nd edition, John Wiley & Sons, New York, 1981.

[13] W.T. Eadie, D. Drijard, F.E. James, M. Roos, B. Sadoulet, *Statistical Methods in Experimental Physics,* North-Holland Publishing Comp., Amsterdam-New York-Oxford, 1982.

[14] *** *Handbook of Applicable Mathematics,* chief editor Lederman W., volume VI: *Statistics,* John Wiley & Sons, New York, 1984.

[15] P.W.M. John, *Statistical Methods in Engineering and Quality Assurance,* John Wiley & Sons, New York, 1990.

[16] D.A. Iordache, "On the Compatibility of some Theoretical Models relative to the Experimental Data", in *Proceedings of the 2nd Colloquium "Mathematics in Engineering and Numerical Physics"* (MENP-2), Bucharest, part 2, pp.169-176, 2002.

[17] W. Meyer, H. Neldel, *Z. Tech. Phys. (Leipzig),* vol. 12, pp. 588, 1937.