Modeling of the minority carriers diffusion in the substrate for SMART Power ICs

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ABSTRACT

In this paper a semi-analytical method is presented to model the electron diffusion in an arbitrary p-substrate. The approach is based on the Green function tecnique. The Green function is derived over a multilayer substrate by solving the diffusion equations analytically in the z coordinate and numerically in the x and y coordinates. Using this technique, the substrate coupling through the parasitic n-well-substrate-n-well bipolars can be accurately analyzed. Preliminary results verify the suitability of the approach.

1. INTRODUCTION

Minority carrier diffusion is a main problem in SMART Power ICs where underground conditions on the output driver stage can lead to significant electron current injection into the substrate. This behavior is exemplified, among others, by half-bridge configurations where negative voltages at the drain terminal of the power DMOS occur during normal operation [1].

There exist several simulators capable of modeling injection of majority carriers into the substrate [2]. However, the only tools capable of evaluating the impact of minority carriers are 2-3D simulators such as ISE DESSIS [1].

These tools incorporate advanced physical models and robust numerical methods for the simulation of most types of semiconductor devices [3]. Due to their numerical complexity, often these methods are computationally inefficient. Thus becomes necessary topological reduction of the structures under test. Another limitation of 2-3D tools is the difficulty of correlating simulation results with immunity problems often present in ICs.

Considering the previous example, the power DMOS n-well / substrate junction can be modeled as the base-emitter of a bipolar (fig. 1) whose collector is any other n-well in the substrate. In this paper, an *ad hoc* approach (called Minority Diffusion Green-function-based Method, MIDGEM), based on [4], is derived which efficiently extracts the beta parameter of this equivalent npn bjt. A new Green function was derived for the minority carrier problem and it is presented in this work. The method, implemented in c++, was verified with full 3D simulations performed in ISE DESSIS.

2. PROBLEM FORMULATION

The continuity equations can be written as [5]

$$\begin{cases} \frac{\partial n}{\partial t} = \frac{\partial n}{\partial t}\Big|_{\mathrm{Diff}} + \frac{\partial n}{\partial t}\Big|_{\mathrm{Drift}} + \frac{\partial n}{\partial t}\Big|_{\mathrm{Rec-Gen}} + \frac{\partial n}{\partial t}\Big|_{\mathrm{Other\_proc}} \\ \frac{\partial p}{\partial t} = \frac{\partial p}{\partial t}\Big|_{\mathrm{Diff}} + \frac{\partial p}{\partial t}\Big|_{\mathrm{Drift}} + \frac{\partial p}{\partial t}\Big|_{\mathrm{Rec-Gen}} + \frac{\partial p}{\partial t}\Big|_{\mathrm{Other\_proc}} \end{cases} \tag{1}$$

$$\begin{cases} \frac{\partial n}{\partial t}\Big|_{\mathrm{Diff}} + \frac{\partial n}{\partial t}\Big|_{\mathrm{Drift}} = \frac{1}{q}\nabla \cdot J_{\mathrm{n}} \\ \frac{\partial p}{\partial t}\Big|_{\mathrm{Diff}} + \frac{\partial p}{\partial t}\Big|_{\mathrm{Drift}} = \frac{1}{q}\nabla \cdot J_{\mathrm{p}} \end{cases} \tag{2}$$

Considering the specific problem under study it is possible to make the following simplifications:

1. in the case of a p-substrate the hole diffusion can be ignored when only the continuity equations for minority carriers in the substrate are considered
2. the Drift component of the electron current density is omitted because electrons are minority carriers and it's assumed a low level injection condition
3. no other processes, like light [5], are present

Under these assumptions the continuity equations become

$$\frac{\partial n}{\partial t} = \frac{\partial n}{\partial t}\Big|_{\mathrm{Diff}} + \frac{\partial n}{\partial t}\Big|_{\mathrm{Rec-Gen}}, \tag{3}$$

where

$$\frac{\partial n}{\partial t}\Big|_{\mathrm{Diff}} = \frac{1}{q}\nabla \cdot J_{\mathrm{n}} = \frac{1}{q}\nabla \cdot (qD_{\mathrm{n}}\nabla n) = D_{\mathrm{n}}\nabla^2 n. \tag{4}$$

In the hypothesis of low injection [7] [8] (3) becomes

$$\frac{\partial n}{\partial t}\Big|_{\mathrm{Rec-Gen}} \cong -\frac{n - n_{\mathrm{p0}}}{\tau_{\mathrm{n}}} = -\frac{\Delta n}{\tau_{\mathrm{n}}}, \tag{5}$$

where n_{p0} is the substrate electron concentration at the equilibrium, so

$$\frac{\partial n}{\partial t} = D_{\mathrm{n}}\nabla^2 n - \frac{\Delta n}{\tau_{\mathrm{n}}}. \tag{6}$$

Assuming steady state (6) becomes

$$D_{\mathrm{n}}\nabla^2 n = \frac{\Delta n}{\tau_{\mathrm{n}}}. \tag{7}$$

For a current source characterized by a minority carriers injection rate ξ (with dimension $carriers \cdot cm^{-3}s^{-1}$) (7) can be rewritten as

$$D_{\mathrm{n}}\nabla^2 n - \frac{\Delta n}{\tau_{\mathrm{n}}} = \xi. \tag{8}$$

Again under the above assumptions, (8) can be solved almost analytically by use of the Green function. In a medium with prescribed boundary conditions, the Green function, $G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}})$, relates the electron concentration at any point $\mathbf{r}$ as a function of an electron source placed at a location $\mathbf{r}_{\mathrm{s}}$. Assuming zero electron concentration at the chip backplane and vanishing normal electric current on the other faces, the electron concentration due to an arbitrary electron source simplifies to

$$\Delta n(\mathbf{r}) = \int_{\mathrm{V}} \xi(\mathbf{r}_{\mathrm{s}}) G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}}) d\mathbf{r}_{\mathrm{s}}, \tag{9}$$

where V is the chip volume region and $\xi(\mathbf{r}_{\mathrm{s}})$ is the function that describes the electron source.
Furthermore, assuming that:

1. the dimension of the contacts is negligible with respect to the substrate geometry, so that the extraction of the Green function can be done neglecting the contacts. (If this condition were not satisfied, the method would be too complex and thereby less attractive.)

2. the current density at a contact is independent on the presence and location of other contacts. (Considering the case of two victim contacts and a source one injecting a current, this condition means that the current collected at one of the two victims is the same if the other contact is not present or, if it is present, it is not connected to any potential.)

The existence of a victim contact adds another condition $\Delta n = 0$ at the surface since all the minority carriers in excess at its surface are collected.
Finally, the minority carriers density is expressed as the sum of two terms. The first term depends on the current source position and the second on the victim contact position

$$\Delta n(\mathbf{r}) = \frac{R_1}{S_{\mathrm{s}}} \int_{\mathrm{S_s}} G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}}) ds_{\mathrm{s}} + \frac{R_2}{S_{\mathrm{v}}} \int_{\mathrm{S_v}} G'(\mathbf{r} \mid \mathbf{r}_{\mathrm{v}}) ds_{\mathrm{v}}, \tag{10}$$

where R_1 and R_2 are the respective carrier density rates and will be described in detail in the next section.
We are not interested in the minority carriers density but in the total current collected at the victim contact, v, due to the current injected at the source contact, s, that from (10) is

$$\begin{aligned} I_{\mathrm{i}} = & \frac{R_1}{S_{\mathrm{s}}} \int_{\mathrm{S_v}} qD_{\mathrm{n}} \frac{d}{dz} \left[\int_{\mathrm{S_s}} G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}}) ds_{\mathrm{s}} \right] ds_{\mathrm{v}} \\ & + \frac{R_2}{S_{\mathrm{v}}} \int_{\mathrm{S_v}} qD_{\mathrm{n}} \left[\frac{d}{dz} \int_{\mathrm{S_v}} G'(\mathbf{r} \mid \mathbf{r}_{\mathrm{v}}) ds_{\mathrm{v}} \right] ds_{\mathrm{v}}. \end{aligned} \tag{11}$$

The first term is zero because the integration in (11) is over the victim contact surface area, S_{v}, and the derivative of $G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}})$ at $z = 0$ is null everywhere but in $(x_{\mathrm{s}}, y_{\mathrm{s}}, 0)$. Due to the discontinuity condition imposed by the victim contact, the second term can be rewritten as

$$\frac{R_2}{S_{\mathrm{v}}} \int_{\mathrm{S_v}} qD_{\mathrm{n}} \left[\frac{d}{dz} \int_{\mathrm{S_v}} G'(\mathbf{r} \mid \mathbf{r}_{\mathrm{v}}) ds_{\mathrm{v}} \right] ds_{\mathrm{v}} = qR_2. \tag{12}$$

Equation (11) becomes $I_{\mathrm{i}} = qR_2$, where the R_2 term is defined in (19), while the total current injected by the source contact is instead $I_{\mathrm{inj}} = qR_1$ so it is possible to express α as follows

$$\alpha = \frac{I_{\mathrm{i}}}{I_{\mathrm{inj}}} = \frac{qR_2}{qR_1} = \frac{S_{\mathrm{v}}}{S_{\mathrm{s}}} \frac{\int_{\mathrm{S_v}} \int_{\mathrm{S_s}} G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}}) ds_{\mathrm{s}} ds_{\mathrm{v}}}{\int_{\mathrm{S_v}} \int_{\mathrm{S_v}} G'(\mathbf{r} \mid \mathbf{r}_{\mathrm{v}}) ds_{\mathrm{v}} ds_{\mathrm{s}}}. \tag{13}$$

Parameter β of the equivalent npn transistor is trivially derived as $\beta = \frac{\alpha}{1-\alpha}$. The two double integrals of (13) can't be analytically solved because of the double infinite summation present in the Green function (see (28)). For this reason a grid is applied to the substrate top surface and the two integrals are numerically calculated for every $\mathbf{r}_{\mathrm{v}}$ and $\mathbf{r}_{\mathrm{s}}$ combination [4],[6]. The resulting coefficients are known as *cross-coupling diffusion coefficients* and they are organized in matrix form.
Because the two Green functions, $G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}})$ and $G'(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}})$, are identical but with a different centering point the numerical calculations are done only once. The source and the victim contacts are then partitioned in sub-elements through the grid previously defined (see fig. 1) and the numerator and denominator of (13) are calculated as the sum of the correspondent cross-coupling diffusion coefficients.

3. DIFFUSION EQUATION SOLUTION

For the relations of (8) to be met, the Green function has to satisfy the following equation

$$\nabla^2 G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}}) - \frac{1}{D_{\mathrm{n}}\tau_{\mathrm{n}}} G(\mathbf{r} \mid \mathbf{r}_{\mathrm{s}}) = -\frac{1}{D_{\mathrm{n}}} \delta(\mathbf{r} - \mathbf{r}_{\mathrm{s}}). \tag{14}$$

In Section 6 a method is shown to derive an expression of the Green function when the victim contact is not present. To enforce this boundary condition another Green function $G'(\mathbf{r} \mid \mathbf{r}_{\mathrm{v}})$ is added to the Green function which solved (14) for the source point centered into the victim point. $G'(x, y, z \mid \mathbf{r}_{\mathrm{v}})$ is a solution of the relative homogeneous equation of (14) and for $(x, y, z) = (x_{\mathrm{s}}, y_{\mathrm{s}}, z_{\mathrm{s}})$

$$\nabla^2 G'(\mathbf{r}_{\mathrm{s}} \mid \mathbf{r}_{\mathrm{v}}) - \frac{1}{D_{\mathrm{n}}\tau_{\mathrm{n}}} G'(\mathbf{r}_{\mathrm{s}} \mid \mathbf{r}_{\mathrm{v}}) = 0 \tag{15}$$

since $G'(x, y, z \mid \mathbf{r}_{\mathrm{v}})$ is centered in the victim point.
In fact, the presence of the victim contact introduces a second discontinuity at the substrate top surface (the first discontinuity is due to the source contact) for $(x, y, z) = (x_{\mathrm{v}}, y_{\mathrm{v}}, z_{\mathrm{v}})$ since for $z = 0$

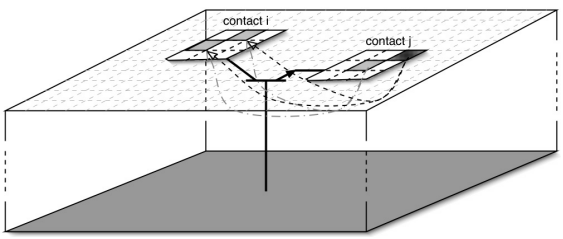

Figure 1: Contact Discretization

the z-derivative of $G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}, \mathbf{r}_\mathrm{v})$ must vanish everywhere but at the victim contact. The first discontinuity is accounted for by $G(\mathbf{r} \mid \mathbf{r}_\mathrm{s})$ while the second by $G'(\mathbf{r} \mid \mathbf{r}_\mathrm{v})$. Therefore, the minority carriers density at the point "**r**" in the substrate can be defined as

$$\Delta n(\mathbf{r}) = \int_\mathrm{V} \xi_1(\mathbf{r}_\mathrm{s}) G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) d\mathbf{r}_\mathrm{s} + \int_\mathrm{V} \xi_2(\mathbf{r}_\mathrm{v}) G'(\mathbf{r} \mid \mathbf{r}_\mathrm{v}) d\mathbf{r}_\mathrm{v}, \tag{16}$$

where ξ_2 must be determined in order to solve the problem. Supposing that both functions ξ_1 and ξ_2 are planar surface sources of a constant and equal distributed minority carrier density rates R_1 and R_2, then the following equations must hold

$$\Delta n(\mathbf{r}) = \frac{R_1}{S_\mathrm{s}} \int_{\mathrm{S_s}} G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) ds_\mathrm{s} + \frac{R_2}{S_\mathrm{v}} \int_{\mathrm{S_v}} G'(\mathbf{r} \mid \mathbf{r}_\mathrm{v}) ds_\mathrm{v}. \tag{17}$$

Let us now define the R_2 parameter in (17) in order to verify all the boundary conditions. The existence of the victim contact at $(x, y, z) = (x_\mathrm{v}, y_\mathrm{v}, z_\mathrm{v})$ imposes not only that the z-derivative of G at this point be different from zero but also that the minority carriers in excess must vanish. This condition can be written as

$$\frac{R_1}{S_\mathrm{s}} \int_{\mathrm{S_v}} \int_{\mathrm{S_s}} G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) ds_\mathrm{s} ds_\mathrm{v} + \frac{R_2}{S_\mathrm{v}} \int_{\mathrm{S_v}} \int_{\mathrm{S_v}} G'(\mathbf{r} \mid \mathbf{r}_\mathrm{v}) ds_\mathrm{v} ds_\mathrm{v} = 0, \tag{18}$$

hence, solving for R_2,

$$R_2 = -R_1 \frac{S_\mathrm{v}}{S_\mathrm{s}} \frac{\int_{\mathrm{S_v}} \int_{\mathrm{S_s}} G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) ds_\mathrm{s} ds_\mathrm{v}}{\int_{\mathrm{S_v}} \int_{\mathrm{S_v}} G'(\mathbf{r} \mid \mathbf{r}_\mathrm{v}) ds_\mathrm{v} ds_\mathrm{v}}. \tag{19}$$

Finally, because of the method used in (18), it remains to be demonstrated that in all the substrate region the minority carriers in excess, Δn, are always greater or equal then zero. The complexity of the Green function prevents a direct verification of this condition. However, we give here an intuition why the conditions actually holds.

In open space, reducing to one dimension, the electron concentration can be expressed as

$$n(x) = n_\mathrm{s} \exp\left(-\frac{|x - x_\mathrm{s}|}{L_\mathrm{eff}}\right), \tag{20}$$

where n_s is the electron concentration at the source point (where a discontinuity is introduced by the abs) and L_eff is the effective diffusion length. Rewriting (17) using the open-space equivalent solution

$$n(x) = n_\mathrm{s} \exp\left(-\frac{|x - x_\mathrm{s}|}{L_\mathrm{eff}}\right) - n_\mathrm{v} \exp\left(-\frac{|x - x_\mathrm{v}|}{L_\mathrm{eff}}\right), \tag{21}$$

where n_v is derived from condition (18).

It is easy to show that (21) has an absolute minimum in x_v. Such minimum is zero due to the condition of (18).

4. EXTENDING THE METHOD

When more than one victim contacts exist, (17) becomes

$$\Delta n(\mathbf{r}) = \frac{R_\mathrm{s}}{S_\mathrm{s}} \int_{\mathrm{S_s}} G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) ds_\mathrm{s} + \sum_{\mathrm{i}=1}^{n} \frac{R_\mathrm{i}}{S_{\mathrm{v_i}}} \int_{\mathrm{S_{v_i}}} G'(\mathbf{r} \mid \mathbf{r}_{\mathrm{v_i}}) ds_{\mathrm{v_i}}. \tag{22}$$

	Max Cputime	Notes
DESSIS	1h 13m	SunFire V120 648Mhz, 2560Mb of ram
MIDGEM	4.7 s	Mac G4 1.33 Ghz, 512MB of ram

Table 1: Cputime comparision for the test structure shown in fig. 2

In this case the computation of R_i coefficients is no longer correct if equation (19) is used. By doing so, the minority carriers in excess would no longer vanish at all victim contacts. Hence, the R_i coefficients must be calculated considering the equivalent multidimensional formulation

$$\begin{bmatrix} R_1 \\ R_2 \\ .. \\ R_\mathrm{n} \end{bmatrix} = \begin{bmatrix} R_\mathrm{s} f(\mathbf{r}_{\mathrm{v}_1} \mid \mathbf{r}_\mathrm{s}) \\ R_\mathrm{s} f(\mathbf{r}_{\mathrm{v}_2} \mid \mathbf{r}_\mathrm{s}) \\ \cdots \\ R_\mathrm{s} f(\mathbf{r}_{\mathrm{v}_\mathrm{n}} \mid \mathbf{r}_\mathrm{s}) \end{bmatrix} \cdot \begin{bmatrix} f(\mathbf{r}_{\mathrm{v}_1} \mid \mathbf{r}_{\mathrm{v}_1}) & f(\mathbf{r}_{\mathrm{v}_1} \mid \mathbf{r}_{\mathrm{v}_2}) & .. & f(\mathbf{r}_{\mathrm{v}_1} \mid \mathbf{r}_{\mathrm{v}_\mathrm{n}}) \\ f(\mathbf{r}_{\mathrm{v}_2} \mid \mathbf{r}_{\mathrm{v}_1}) & f(\mathbf{r}_{\mathrm{v}_2} \mid \mathbf{r}_{\mathrm{v}_2}) & .. & f(\mathbf{r}_{\mathrm{v}_2} \mid \mathbf{r}_{\mathrm{v}_\mathrm{n}}) \\ .. & & & \\ f(\mathbf{r}_{\mathrm{v}_\mathrm{n}} \mid \mathbf{r}_{\mathrm{v}_1}) & f(\mathbf{r}_{\mathrm{v}_\mathrm{n}} \mid \mathbf{r}_{\mathrm{v}_2}) & .. & f(\mathbf{r}_{\mathrm{v}_\mathrm{n}} \mid \mathbf{r}_{\mathrm{v}_\mathrm{n}}) \end{bmatrix}^{-1} \tag{23}$$

where

$$f(\mathbf{r}_{\mathrm{v_i}} \mid \mathbf{r}_{\mathrm{v_j}}) = \frac{1}{S_{\mathrm{v_i}}} \int_{\mathrm{S_{v_j}}} \int_{\mathrm{S_{v_i}}} G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) ds_{\mathrm{v_i}} ds_{\mathrm{v_j}}. \tag{24}$$

Considering the open-space expression of the diffusion law it is possible to verify that also in this case the method used in (23) ensures that Δn is always greater or equal than zero in all the substrate region.

This extended method requires the inversion of the f matrix, as shown in (23). The complexity of doing this is cubic in the number of victim contacts.

5. RESULTS

In this section a comparison is presented between the results obtained simulating the electron diffusion on a particular structure with ISE DESSIS and with MIDGEM. It must be clarified that while MIDGEM requires only the contacts to be meshed (and it

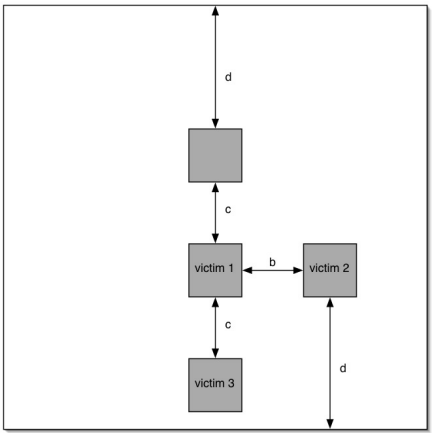

Figure 2: Test Structure

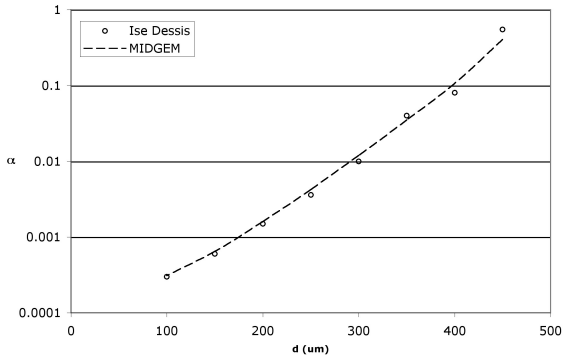

Figure 3: α (see eq. 13) as a function of d for the structure of fig. 2 without victim2 and 3 contacts

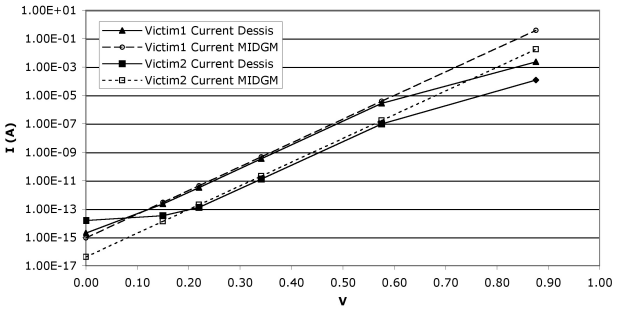

Figure 4: Collected current at victim1 and 3 for b=c=200 μm and d=300 μm as a function of the voltage applied to the injecting n-well/substrate junction

must be done only once if the chip geometrical and electrical characteristics don't change), in DESSIS the entire substrate is meshed (and, for optimization, if a single contact is varied, then the entire problem has to be recomputed). This is why MIDGEM is more computationally efficient (tab. 1).

The first tests are performed on a lateral npn fabricated using two n-wells on a p-substrate, whereby the distance between the wells is parameterized as shown in fig. 2. The dimensions of the substrate are set to 1000x1000x300 μm doped with a boron concentration of 10^{16}cm^{-3} and a back contact modeled as a conductive surface. The n-wells are modeled as a box of 100x100x10 μm doped with a phosphorus concentration of 10^{20}cm^{-3} and a surface contact at the top modeling the metal contact. The n-wells are denominated "injecting" and "victim1" ("victim2" and "victim3" at first are not included).

Fig. 3 reports the ratio between the collected and injected currents as a function of d. The error between DESSIS and MIDGEM is no more than 32%. Moreover, since the contacts are modeled as simple surfaces, the nearer the contacts the higher the lateral component of the injected current. A higher collected current from the n-well side-walls may therefore affect the results.

Other results are presented in fig. 4 where victim2 is removed from the test structure: the method is pretty accurate (50% of error) also in the case of contacts very near the chip sidewalls (50 μm). As expected, the diffusion law dominates for injected current lower than some milliamperes and the structure acts like a bipolar. For bigger currents, the resistive nature of the substrate becomes more important. This is generally true for commonly-used smart-power technologies as reported in [1].

The structure was also tested without contact3 to verify an asymmetric case to compare the approach proposed in Section 3, let us call this MIDGEM1, and the one presented in Section 4, let us call this MIDGEM2. In this case, the current collected by each of the contacts is

$$I_{\text{victim}_\text{i}} = \frac{\beta_{\text{victim}_\text{i}}}{1 + \sum_{\text{j}=1}^{n} \beta_{\text{victim}_\text{j}}} I_{\text{injected}}, \tag{25}$$

where "n" is the number of victim contacts considered. MIDGEM1 clearly introduces a consistent error in the calculation of α referred to the second victim contact when the two contacts are near and particularly in the case of d=400 μm. MIDGEM2, instead, as shown in fig. 6, induces a maximum error of about 20%.

In SMART Power ICs the power transistors act like sources and usually the only contacts that are near them are those of other power-transistors. In this case the error introduced in nearby areas is compensated by low diffusion coefficients in far regions which are very well estimated. Hence the overall error is generally limited. In these cases MIDGEM1 could be a viable alternative to speed up the extraction process.

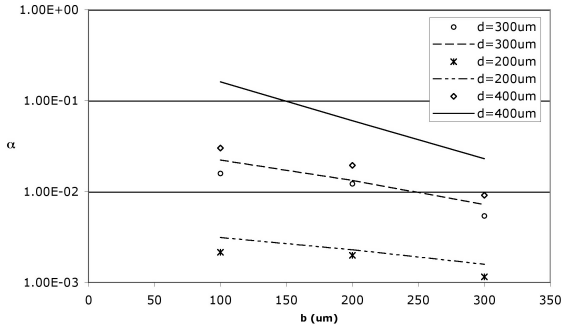

Figure 5: α as a function of the distance d for the victim 2 contact of the structure of fig. 2 using the MIDGEM1 method

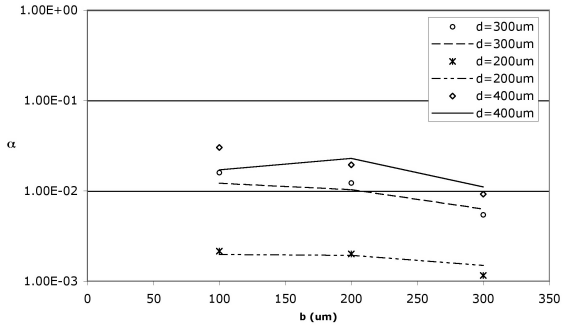

Figure 6: α as a function of the distance d for the victim 2 contact of the structure of fig. 2 using the MIDGEM2 method

6. CONCLUSIONS

In this paper, a novel technique based on a Greens Function approach to substrate analysis have been proposed for efficient evaluation of parasitic electron diffusion in SMART Power ICs.
Preliminary results demonstrate the validity of the assumptions and the good accuracy of this method. Due to the efficiency of the Greens Function approach, the proposed technique can be used in what-if analyses as well as in optimization, including placement and routing. Finally, the tool can be useful in determining *a priori* immunity of the circuit to this type of interferences, thus helping control yield and minimizing design risks.

7. ADDITIONAL AUTHORS

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APPENDIX: Green Function Derivation

Starting from (14), let us separate the variable and express $G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) = X(x, x_\mathrm{s})Y(y, y_\mathrm{s})Z(z, z_\mathrm{s})$. The equation becomes

$$YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2} - \frac{1}{D_\mathrm{n}\tau_\mathrm{n}}XYZ = -\frac{1}{D_\mathrm{n}}\delta(x - x_\mathrm{s})\delta(y - y_\mathrm{s})\delta(z - z_\mathrm{s}) \quad (26)$$

Choose $X = \cos(\frac{m\pi x}{L_\mathrm{x}})$ and $Y = \cos(\frac{n\pi y}{L_\mathrm{y}})$ where $m = 0, 1, 2, ..$ and $n = 0, 1, 2, ..$, in order to satisfy the relative homogeneous equations and the boundary condition of zero normal current on the side walls. Equation (26) becomes

$$\sum_{\mathrm{m}=0}^{\infty}\sum_{\mathrm{n}=0}^{\infty}\cos\left(\frac{m\pi x}{L_\mathrm{x}}\right)\cos\left(\frac{n\pi y}{L_\mathrm{y}}\right)\left\{\frac{d^2Z}{dz^2} - \gamma_\mathrm{mn}^2 Z\right\} = -\frac{1}{D_\mathrm{n}}\delta(x - x_\mathrm{s})\delta(y - y_\mathrm{s})\delta(z - z_\mathrm{s}) \quad (27)$$

where $\gamma_\mathrm{mn} = \sqrt{\left(\frac{m\pi}{L_\mathrm{x}}\right)^2 + \left(\frac{n\pi}{L_\mathrm{y}}\right)^2 + \frac{1}{D_\mathrm{n}\tau_\mathrm{n}}}$.
The derivation then follows exactly what done in [4] so it's not presented here. The final expression is

$$G(\mathbf{r} \mid \mathbf{r}_\mathrm{s}) = \sum_{\mathrm{m}=0}^{\infty}\sum_{\mathrm{n}=0}^{\infty}\frac{C_\mathrm{mn}}{D_\mathrm{n}L_\mathrm{x}L_\mathrm{y}\gamma_\mathrm{mn}}\frac{\mathrm{B_N}tanh(\gamma_\mathrm{mn}d) + \Gamma_\mathrm{N}}{\mathrm{B_N} + \Gamma_\mathrm{N}tanh(\gamma_\mathrm{mn}d)} \times \cos\left(\frac{m\pi x}{L_\mathrm{x}}\right)\cos\left(\frac{m\pi x_\mathrm{s}}{L_\mathrm{x}}\right)\cos\left(\frac{n\pi y}{L_\mathrm{y}}\right)\cos\left(\frac{n\pi y_\mathrm{s}}{L_\mathrm{y}}\right) \quad (28)$$

where $C_\mathrm{m,n}$ equals 1 for m=n=0, 2 for m=0 and $n \neq 0$ or $m \neq 0$ and n=0, 4 otherwise.