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Uncertainty Quantification for Robust Topology Optimization of Power Transistor Devices

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In this paper we focus on incorporating a stochastic collocation method (SCM) into a topological shape optimization of a power semiconductor device including material and geometrical uncertainties. Such geometrical and material variations, which result predominantly from lithography proximity and process imperfections, have a direct impact on yield and performance of these devices. This results in a stochastic direct problem and, in consequence, affects the formulation of an optimization problem. Specifically, we deal with the robust optimization of a power transistor in order to minimize the current density overshoots, since the change of the shape and topology of a device layout is the proven technique for the reduction of a hotspot area. The gradient of a stochastic cost functional is evaluated using the topological asymptotic expansion (TAE) and the continuous design sensitivity analysis (CDSA) with the SCM. Finally, we show the results of the robust optimization for the power transistor device, which is an example of a relevant problem in nanoelectronics, but which is also used widely in the automotive industry.

Index Terms—Design optimization, nanoelectronics, power transistors, robustness, topology, uncertainty quantification.

I. INTRODUCTION

The power semiconductor devices play a key role in efficiently exploiting resources and energy in power electronics with respect to both an energy harvesting and distribution as well as in applications for automotive industry. In fact, due to the proximity effect in lithography and several process variations, the physical domain of power devices made of several thousands of parallel channel devices, cannot be determined precisely. In particular, the imperfections in manufacturing processes related primarily to sub-wavelength lithography, lens aberration, and chemical-mechanical polishing belong to the most important variation issues, since they directly influence both the yield and performance [15]. In consequence, they determine also the acceptability, reliability and profitability of power electronic systems, which depend mainly on variation tolerances, e.g., [7]. This, in turn, is especially important in automotive applications that require the handling of electro-thermal operational constraints to the design of both components and systems. In this context, the localized imperfections of the die inside may result in the formation of a ‘hot spot’ (see Fig. 7) that rapidly heats and leads to the destruction of a power device, e.g., [1] and [12].

The problem of a thermal instability has been known to the automotive industry since the year 1997 when the very fast switching MOSFET devices were introduced onto the market [12]. This phenomenon, which is a main reason for the reduction of the safe operating area, results from a temperature instability mechanism induced by an uneven distribution in drain current as a side effect of the progressive die size and the process scaling down [1]. However, the positive temperature coefficient in a wide range of drain currents, which causes a kind of second breakdown phenomenon, is related to the geometrical and physical parameters of a power device; see [1] and [4]. From this point of view, it is possible to reduce a thermal instability by optimizing the geometry within the device layout while taking both the conductive power losses and robustness into account. Therefore, in this work we apply the SCM [14] with the Polynomial Chaos Expansion (PCE) for the assessment of the reliability and robustness of a design w.r.t. uncertain parameters from manufacturing, e.g., tolerances variations, described by random variables. This solution allows for the efficient calculation of statistical moments and additionally yields directly a response surface model, which can be easily incorporated in a robust topology optimization, e.g., [9].

![Fig. 1. Structure in a power transistor device [11].](image)

A novelty of this paper is to incorporate the SCM into the topology derivative method in order to eliminate the hot-spot phenomena while taking the geometrical and material variations into account. The latter is an important requirement in real engineering applications, where designers ought to consider some manufacturing tolerances during the optimization process.

II. MODEL DESCRIPTION

The special construction of a power device, shown in Fig. 1, is considered here as a case study. The source and drain contacts are placed on the top of the design. It consists of several thousands of parallel channel devices, where the current to drain and away from the sources of the individual channel is transported by complex series of metal stripes and via patterns. In this case, a drift-diffusion model is much too expensive to calculate a complicated current-flow pattern.
Therefore, the electro-thermal coupling problem of a power transistor has been formulated and solved at MAGWEL in an ab-initio self-consistent manner [11]. Accurate modeling of metal layers as required for advanced integrated BCD (Bipolar-CMOS-DMOS) technologies has been obtained by the application of a high spatial resolution. Moreover, the simulator uses a well-adopted mesh for the substrate, which is important for the simulation of the temperature. Joule self-heating and heat flow in metal is modeled together with nonlinear temperature-dependent electrical conductivity \( \sigma = W_\alpha \sigma_0 \) with \( W_\alpha \) being the layer size), thermal conductivity \( \kappa \) and thermal capacitances \( C_\rho \) of materials. Thus, finally the flow of currents \( \mathbf{J} \) is governed by the coupled, random-dependent PDEs on \( \mathbf{x} \in \Omega \subset \mathbb{R}^3 \)

\[
\begin{align*}
- \nabla \cdot ( \varepsilon \mathbf{E}) &= \rho, \\
\nabla \cdot \mathbf{J} + \delta, \rho &= 0, \\
\mathbf{J} &= \sigma \mathbf{E}, \\
\delta \mathbf{U} &= \nabla \cdot \mathbf{Q} + \mathbf{Q},
\end{align*}
\]

imposed with suitable boundary/initial conditions [11]. Here, \( \rho, \varepsilon \) denote the charge density and the permittivity. \( \mathbf{E} \) is the electric field, while \( U = C_\rho (T - T_0), \mathbf{Q} = -\kappa(T) \mathbf{V} \mathbf{T} \) and \( \mathbf{Q} = \mathbf{E} \cdot \mathbf{J} \) denote the heat flux, where \( T_0 \) is a room temperature, the heat flow and self-heating due to Joule’s law. As a result of such an approach, every electric transport inside the MOS channels is dealt with a compact model, e.g. \( I_{DS} = f(V_{DS}, V_G) \). Likewise, the heat generated in the channel is also calculated from the channel resistance by \( \mathbf{Q} = V_{DS} \mathbf{I}_{DS}(V_{DS}, V_G) \). By this powerful novel approach it is possible to solve such a big system.

### III. UQ FOR THE STOCHASTIC FORWARD PROBLEM

The method of the (generalized) polynomial chaos (g/PC), first proposed by Norbert Wiener [16] has recently found a broad application in electrical engineering to assess the reliability and robustness of design with respect to uncertain parameters, e.g. [2] and [9]. For the UQ analysis we substitute some parameters \( \mathbf{p} = (p_1, \ldots, p_n) \) in model (1) by independent random variables \( \xi \), defined on some probabilistic space \((\Theta, \Sigma, P)\). Then, its response \( u \) can be expanded in the truncated PC series [14]

\[
u(s, \xi) = \sum_{k=0}^{K} a_k(s) \Omega_k(\xi),
\]

where \( \Omega_k \) are orthogonal basis polynomials such that \( \mathbb{E}[\Phi_k \Phi_l] = \mathbb{E}[\Phi_k^2] \delta_k^l \) w.r.t. distributions of \( \xi \), where \( <\Phi_k, \Phi_l>: = \mathbb{E}[\Phi_k \Phi_l], s \) refers to the nonprobabilistic variables, e.g., design variables. \( \mathbb{E}[] \) and \( \delta_k^l \) denote an expected value and the Kronecker delta, respectively. To calculate the a priori unknown coefficients \( a_k \) a pseudospectral approach with suitable quadrature rules chosen has been used

\[
a_k(s) = \frac{1}{Y_k} \mathbb{E} [u(s, \xi) \Phi_k(\xi)] = \frac{1}{Y_k} \sum_{i=1}^{N_q} u(s, \xi^{i(n)}) \Phi_k(\xi^{i(n)}) w^{i(n)},
\]

where \( Y_k = \mathbb{E}[\Phi_k^2] \) are the normalization constants of the basis, \( (\xi^{i(n)}, w^{i(n)}), n = 1, \ldots, N_q \) are nodes with their corresponding weights. Thus, the basic idea of this method is to provide the deterministic solution at each quadrature grid point \( \xi^{i(0)} \).

Fig. 2. UQ of I(drain) due to variations of the Metal3 thickness, modeled by a Gaussian distribution with 10% variation around a mean of 1\,\mu m.

Fig. 3. UQ of T(probe) due to variations of \( \sigma \) in Metal3, modeled by a uniform distribution with 15% variation around a mean 20 MS/m.

Given the PCE coefficients \( a_k \), we obtain an approximation of the mean value \( (\mu_k) \) and the variance \( (\sigma_k^2) \) [14], shown on Fig. 2 and 3

\[
\mu_k(s) = a_0, \quad \sigma_k^2(s) = \sum_{s_k} a_{s_k}^2(s) \mathbb{E}[(\Phi_k^2)].
\]

As a result of this expansion both the global, the so-called variance-based, and local sensitivity analysis, shown on Fig. 4, can be carried out.

Fig. 4. Local sensitivity analysis of I(drain) versus chosen parameter \( p(\xi) \).

From a robust topology optimization viewpoint, especially the first order probabilistic expansions is essential. The way how to find the PCE for the topological sensitivity, which is a clue of the proposed algorithm for a robust design,

\[
\frac{d \mu_k}{d s} = \frac{d a_0}{d s}, \quad \frac{d \sigma_k^2}{d s} = \sum_{s_k} \frac{d a_{s_k}^2}{d s} \mathbb{E}[(\Phi_k^2)]
\]

will be shown in the next section.

### IV. STOCHASTIC OPTIMIZATION PROBLEM

To robustly and efficiently deal with the topological shape optimization of a power transistor device under uncertainties in 3D, a new algorithm for robust sensitivity-based topology design is proposed.
A. Topological Gradient and its Expansion

The concept of a topological derivative (TG) comes from structural engineering [13] and more recently has found a broad application in deterministic, electromagnetics problems, e.g., [6] and [10]. The TG asymptotic expansion can be derived for a broad class of the 2D/3D problems [8]. Let $j(\Omega) := F(\psi_0)$ denote an arbitrary objective functional to be minimized with $\psi$ being the solution to a given PDE problem on domain $\Omega$. Further, let for $d > 0$, $\Omega_d := \Omega \cup B(x_0, d)$ be the subset of $\Omega$ after removing $B(x_0, d)$ being a small hole with the center $x_0$ and a radius $d$. Then, the variation of the topological criterion is given by its asymptotic expansion [8]

$$ j(\Omega_d) - j(\Omega) = f(d) g(x_0) + o(f(d)), \quad \lim_{d \to 0} f(d) = 0, \quad f(d) > 0. \quad (7) $$

In other words, to minimize the criterion $j$ one needs to create infinitely small holes at some points $\mathbf{x}$, where the topological sensitivity $g(\mathbf{x})$ is negative taking the optimality conditions and area/volume constraints into account [3].

B. The Random-Dependent Objective Functional

To minimize the current density overshoots, the random-dependent cost functional w.r.t. the dissipation power on $D_1 \subset \mathbb{R}^2$ with a source $h$ defined on $D_2 \subset \mathbb{R}^2$ will be given by

$$ F_\psi(\psi(\mathbf{u})) = \int_{\Omega_0} Q(-\nabla \phi(\mathbf{u}), \mathbf{u}) d\mathbf{x} + \int_{\Omega_2} h(\psi(\mathbf{u})) d\mathbf{x}, $$

where $\mathbf{u} = (\mathbf{x}, s, \xi)$ and a function $p$ denotes a normal component of the electric field strength. In general, we consider here a random optimization problem with deterministic mass/volume and box constraints.

C. Shape and Topological sensitivity for a power device

Let piecewise constant functions such as $\beta(\mathbf{x})$ and $\gamma(\mathbf{x})$ been given as

$$ \beta(\mathbf{x}), \gamma(\mathbf{x}) = \begin{cases} \beta_i, \gamma_i & \text{if } \mathbf{x} \in D_i \setminus B, (\mathbf{x}, d) \\ \beta_i, \gamma_i & \text{if } \mathbf{x} \in B, (\mathbf{x}, d) \end{cases} \quad (9) $$

where a subscript $i$ refers to domains $D_1$ and $D_2$, respectively. Furthermore, for the simplicity, we consider the $n$-th realization of random parameters in our model. Then, the topological sensitivity can be defined by [3], [5] and [8]:

$$ 2D : F(d) - F(0) = -2\pi d^2 \Re \{2 \{p(\psi_{*}) p(\lambda_{*})\} + o(d^2) \} \quad (10) $$

$$ 3D : F(d) - F(0) = -4\pi d^3 \Re \{ \frac{(\gamma_{*} - \gamma_{*})}{(\gamma_{*} - 2\gamma_{*})} \} - \nabla \phi(\mathbf{u}) \cdot \nabla \phi(\mathbf{u}) + o(d^3) \quad (11) $$

In (8) it has been assumed that a power device is driven by voltage. In case of a current source problem one can apply Tellegen’s theorem or directly the TG formula [5]. Since the objective functional corresponds to the dissipation power analyzed in a time-harmonic state space analysis, a dual problem is the rescaled version of a primary problem, thus the adjoint variable $\lambda = \phi', \phi$ where $\phi$ represents the scaling. From (10) and (11) one can easily extract information on a shape sensitivity as well [3].

D. Robust Topological Shape Optimization

Finally, we formulate the shape optimization in the framework of the robust bi-objective optimization [9] using the expectation and the standard deviation values

$$ \min : \mathbb{E}[F_\psi(\psi)] + \eta \mathbb{V}[F_\psi(\psi)] \quad (12) $$

s.t. : $K(\psi^{***}) = \eta^{***}$, $n = 1, ..., N_s$, $area/vol(D_i) \leq m, i = 1, 2, 3$, $\nu_{max} \leq \nu \leq \nu_{min}, j = 1, 2, 3$, where $\eta = 3$ is a prescribed parameter, $K$ denotes the stiffness matrix calculated at $N_4$ quadrature grid points. To calculate the total derivative of the robust bi-objective functional based on a forward model analysis in collocation points, one needs to find a PC expansion using (2) and (3) to the topological sensitivities expressed by (10) and (11).

V. NUMERICAL EXPERIMENTS

As a case study we consider a structure of a Power MOS device, shown on Fig.1. More specifically, we aim at the robust topological shape optimization of both Matel3 layer and the area of both pads (source and drain) in order to eliminate hot spots phenomena. Thus, finally we deal with the stochastic shape and source optimization problem. However, besides results for the robust topology optimization (RTO), for the purposes of comparison we show also the effect of the deterministic topology optimization (DTO).
removed. The current density (CD) and the hot spots phenomena treated here as violations of the CD in the Contact layer for the initial model are shown on Fig. 7.

![Fig. 7: Initial Model with Contact Layer](image1)

In turn, the results for the DTO and the RTO, when taking the CD with the violation threshold $|J_{\text{cd}}| = 1.16 \times 10^{-6} \text{A/m}^2$ in the Contact layer into account is presented in Fig. 8.

![Fig. 8: CD in Contact Layer after optimization](image2)

In both cases, the temperature, shown on Fig. 9, has been also decreased, for the DTO it became 7.4 °C, while for the RTO the value is 8.0 °C. Finally, we present also the course of the total resistance ($R_{\text{tot}}$) and the total power (P) during the optimization in Fig. 10 and Fig. 11, respectively.

![Fig. 9: Distribution of T in optimized models](image3)

![Fig. 10: Total resistance in a function of iteration](image4)

![Fig. 11: Total power in a function of iteration](image5)

VI. CONCLUSION

In our paper we conduct both the deterministic and stochastic optimization. We successfully implemented our algorithm in Python for the Magwel software. For both kinds of the optimization, the hot spots phenomena have been totally removed. Also the temperature in the Contact layer has been significantly decreased. Our methodology for the stochastic optimization can be also used for the different power device technology like the low power MOS device.

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REFERENCES