Looking for Quality in TCAD-Based Papers

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During the last few years, we have seen an increasing number of submissions of "physics-based simulation only" papers to the IEEE Transactions on Electron Devices (T-ED). The popularity of such papers may be explained by the fact that the nowadays widespread Technology Computer Aided Design (TCAD) tools are a significant and welcome boost to creativity in the electronic device community. In fact, TCAD tools allow researchers to explore and optimize device structures without being burdened by technology concerns in terms of availability, cost and time delay.

To paraphrase the editorial by Doug Verret "Touchstones of a Quality Compact Model" (IEEE Transactions on Electron Devices, Vol. 56, no. 11, November 2009), while we intend to continue to encourage original submissions of TCAD-based papers, we are keenly interested in maintaining and even improving their quality by stimulating *more high-quality submissions, which immediately begs the question "What is the definition of high quality?"* In this editorial, we try to answer, at least partially, to this question.

While fabrication, at least in perspective, should be the ultimate goal of any electronic device or material design, the lack of experimental verification does not necessarily imply, by itself, that the quality of a paper is unsatisfactory. In the past, we had great visionary papers proposing new devices with the support of simple analytical models, without the backing of experimental data. Think about the evolution of field-effect transistors and of heterojunction bipolar transistors, whose idea came well before technology were able to provide working realizations. If only simulations entirely supported by experiment were considered as acceptable, there would not be much point to use physics-based modelling to explore new materials and device designs.

Nevertheless, authors should take care to include in their simulation papers a realistic appraisal of the technological issues involved, and to give thoughts or discussion on the validity of the simulation approach used. Optimally, they should provide some evidence that their simulation approach reflects reality, if possible through an (also partial) measurement-based validation. Since, in most fields of semiconductor and vacuum electronics, technology is expensive and often out of the authors' reach, we are aware that direct experimental validations are often difficult to obtain.

To provide some more specific guidelines on quality criteria for "physics-based simulation only" papers, it is helpful to divide them into a number of somewhat different classes (examples are taken from the field of semiconductor electronics, but similar remarks hold for vacuum electronic devices):

1. Papers devoted to advances in physics-based simulation techniques in terms of numerical schemes or simulation paradigms, or to the application of numerical simulations in new contexts, e.g. within the framework of multi-physics TCAD tools; application to specific devices may be presented as case studies demonstrating the capabilities of the techniques proposed.

   ➔ Such papers are well within the scope of T-ED only if they propose significant advances of TCAD tools from a physical or technological perspective, and/or a real breakthrough from a computational standpoint, including benchmarks between the proposed schemes and existing simulation methods, rather than presenting correct but incremental improvements on numerical or programming approaches. In the latter case, journals that are more appropriate exist for submission.

2. Papers investigating new material classes through ab-initio simulation techniques and/or exploring entirely new devices based on accurate and powerful simulation tools, like Monte Carlo or Non-Equilibrium Green's Function (NEGF), sometimes with suggestions on how such structures could be realized from a technological standpoint.

   ➔ Papers falling in this category often address material classes whose technology is still under development (think about the countless varieties of 2D chalcogenides). For such papers, the issue of technological realization is sometimes ill posed – their very purpose is to trace a path to the development of technology with the help of simulations. However, class 2) papers should also provide a critical appraisal of the advanced simulation tool used – trademarks like Monte Carlo are not always implying, by themselves, high accuracy. Similar considerations hold for Density Functional Theory (DFT) codes, where different functionals can yield wildly different results, particularly in the context of 2D materials.

3. Papers devoted to the TCAD tuning and optimization of existing, already proposed and often well-established devices in terms of performance (e.g. the breakdown voltage, the threshold voltage, the subthreshold slope…), without an experimental evidence demonstrating that such an optimization is actually effective or feasible or convenient from a technological standpoint.

   ➔ About such papers, it is well known that a meaningful TCAD "fine optimization" of geometries and doping profiles requires very good knowledge and control of the material technological and physical parameters affecting the TCAD results. Moreover, optimization or tuning studies should take into consideration that process variability does not often allow, in practice, a fine control of the optimization variables. Therefore, such optimization exercises are intrinsically critical, and should include direct or indirect experimental evidence of the technological steps required to implement the proposed structures, together with an assessment of the accuracy of the TCAD model used against other simulations or experiment.

4. Papers that propose variations of emerging device structures (that sometimes hardly exist in the laboratory), or even entirely new devices, with a claim of improved performances, on the basis of standard TCAD simulations carried out through commercially available numerical tools.

   ➔ Such papers exploit standard TCAD tools to devise new device concepts or potentially interesting variations of already proposed devices. Even in this case, the question is, how revolutionary is the new device proposed? How technologically feasible is the suggested optimized structure? How accurate is the TCAD model used? Good papers should offer a satisfactory answer to those points. For example, designing a new tunnel-FET using commercial TCAD codes will certainly push the available non-local tunneling models towards (or over) their limits of validity and would require an extremely critical discussion, which is unlikely to be successful without experimental data or resorting to more advanced approaches such as NEGF.

5. Papers where analytical or quasi-analytical techniques for the solution of approximated forms of the drift-diffusion model (often reduced to the Poisson equation) are used to replicate, with a certain degree of accuracy, results from standard TCAD tools, frequently with application to advanced devices (e.g. nanowire FET) whose analysis can exploit geometrical symmetries.

   ➔ Papers belonging to this class should also be considered with care, in particular when they use standard, well-known modeling approaches. Even if they are correct, the amount of novelty they provide should be critically estimated. If a result can be obtained with a commercially available TCAD tool, the added value of some analytical *tour-de-force*, however accurate, is doubtful, unless of course the authors can demonstrate that the analytical approach is indispensable. This may happen e.g. when the structure to be analyzed is too large to be investigated in a reasonable CPU time by brute-force TCAD, or if a statistical Monte Carlo parameter study has to be performed, that is too CPU intensive on the original TCAD model.

6. Compact modeling papers of emerging devices (sometimes hardly existing in the laboratory), the compact model being validated by TCAD simulations, with the purpose of analyzing / optimizing / comparing circuit-level (analog or digital) performances of the devices considered.

   ➔ These papers should often be better submitted to other journals, like, for example, the *IEEE Journal on Exploratory Solid-State Computational Devices and Circuits*. In some cases, papers belonging to this class, though formally correct, have little practical relevance, since the circuit application they consider is sensitive to features of the device technology that cannot be correctly captured by a compact model, in particular when the compact model is identified through TCAD simulations made on ideal devices. Examples are papers where figures of merit of analog circuit performance (e.g. distortion for a power amplifier), that critically depend on technological implementation and device parasitic elements, are evaluated and optimized on the basis of compact models of ideal devices which, sometimes, still lack experimental demonstration.

Last but not least, TCAD-based papers should provide an as complete as possible list of the simulation parameters (geometrical, material, transport, discretization…) and of course a clear indication of the simulation tools used. Ideally, they should allow the reader to reproduce the presented results by using the same or a comparable piece of software. We do realize this is a quite formidable task for the authors to carry out; however, the CAD projects associated with a paper can be made available to the readers through the IEEE DataPort repository (see https://ieee-dataport.org/). Due to the present standardization of TCAD tools, part of the audience will be able to directly run the project and, if not, full information on the models and parameters can be recovered from the project files. Moreover, if models are implemented through a number of standard programming languages, the relevant code can be linked to the paper via the IEEE Code Ocean (see https://codeocean.com/) where readers can run it on a virtual machine.

From the above remarks, the quality of papers entirely based on TCAD simulations appears to ultimately depend on a number of factors: the accuracy of the techniques used; the novelty of the results provided; the fact that the structures proposed are realistic from a technological standpoint. Experimental data should be used whenever available to tune the model parameters and provide an (at least partial) verification of the results. As already stressed, an added value is moreover provided by the authors making supplemental material available in terms of the source code of the TCAD models. Good quality "simulation only" papers should strive to find a satisfactory balance between all these factors.

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