Sooner and Better, Perfection in Compromise and Getting it Right First Time : Some Hopes and Realities of Simulation in Industry

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***Abstract*—We discuss some of the considerations for industrial R&D. From simulation through fabrication to test, we need to make approximations and deal with limitations and reality differing from what is in our model. We shall touch on what makes for a good R&D flow to get it right**

Keywords—industry, simulation, photonic components

I. INTRODUCTION

The history of manufacturing has developed from artisan hand crafted products through division of labour and automation and final, with semiconductors at least, to massively parallel manufacturing at wafer scale. In some aspects though, simulation and manufacture of optoelectronic devices still uses a group of veteran artisans, with decades of experience, hand crafting devices with intuition and focused simulation along with tweaking and adjustment of processes. It has long been stated that grand unification in photonics (as can be achieved with the silicon electronics industry) is challenging since electrons are grey, whereas photons are diverse in; colour, phase and polarisation, and the range of materials to make them equally so. Approaches to automate the design process are greatly aided by Moore's law watching/driving computing power which underpins the ability to perform detailed self-consistent simulation that was previously unimaginable. Machine learning and AI optimisation and automation techniques have recently gained popularity, especially in certain areas such as multi-parameter optimisation and simulation code generation. The simulation is, at best, as good as the information fed in to the model.

II. SIMULATION IS ALL WE NEED

The basic requirement for modelling is the ability to build an analogy of the device to explore a single parameter. This may even be qualitative in nature, if it is to be augmented with a manufacturing DoE. The location of any 'cliff edge' (sharp drop in performance as a design parameter is changed) and the width or area of an optimum can be established. Moving on from this, we can go all the way to building a self-consistent model that can allow the devices to be completely optimised. In this case, if we truly believe the model, we do not even need to consider a DoE or a process run but we can just compare the optimum against product specification. In principle, this can eliminate months of R&D fabrication and test and allow the customer to make an informed decision to move directly to new product introduction (NPI).

Many software companies are building ever more complex models where almost all conceivable physics can be turned on, and examples are given where results in papers are dutifully recreated. To modify these examples as a starting point for device simulation appears to be sensible but there is some caution needed - deviating from these examples may result in unexpected results because the fitting includes entire material libraries stretching back decades and often many more parameters then there are degrees of freedom in the data. In practice, we tend to over-write built in database parameters based on local knowledge using historic device results. We do not even need agree word-wide on these parameters. An example is something that should be pretty simple to understand and agree on e.g. bandgap. A machine grows the semiconductor using flow rates to generate a calibration sample that is measured using photoluminescence. This then dictates adjustments to that layer when it is used in a full QW stack (based on read-across from previous device performance) and we can finally measure spontaneous emission (SE) or gain on those devices over some current range. Knowing the absolute bandgap is not important. On the other hand, a simulation tool often takes atomic compositions and calculates bandgaps. Many additional parameters are used for carrier recombination, leakage, spectral shifts, broadening, etc. contribute to generating SE and gain spectra over some carrier densities. Knowing the absolute bandgap is again not important in itself.

Even in modern times with the exponential growth in computing resource, a fully self-consistent model in terms of carrier dynamics, optical field and temperature, with sufficient 3D resolution is computationally expensive. Nonetheless, a standard desktop machine can handle a large amount of the required simulation for everyday needs. One interesting aspect of modern design is the proliferation of Python based libraries for simulation and machine learning, often in open source format, courtesy of countless thousands of PhD students and academic groups. This lowers the barrier to entry for many companies, and new students. For inverse design approaches, large numbers of designs need to be ran to build the training set and so full simulation is no longer practical. In this case we prefer to use some rapid or home-made compact model that is built for speedy generation of the large numbers of training sets. These models have as little physics as needed to do the job and should compromise everything for speed. The machine learns from these to magically give us our target design.

III. DON'T MODEL IT, MAKE IT

Companies and institutes that possess fabrication facilities have an engineering driven approach at their disposal. This constitutes a more iterative approach, based on repeated cycles of manufacturing. Pushing back against extensive or prolonged simulation is the ability to use a short cycle time to rapidly fabricate devices and test them to truly believe the real performance. In this approach, the combination of the fabrication and the design are intertwined to give the results on the devices that can actually be made, rather than those that are idealised. The materials, misalignments, shape loss through lithography, etch, deposition, regrowth etc must be considered in the final product anyway.

With all these varied tools at our disposal, and many forms of compromise to take, we can discuss what approach can be taken to develop world class devices as fast as possible.

IV. We Don’t Test What We Designed, But What We Made

To understand how the device works and verify any simulation output or customer specification is ‘merely’ a case of testing it. Can we take some equipment in the lab, poke and prod at the chip itself to get all the answers? For example an absorption modulator chip requires a carrier with rf strip-line and termination to make a more complex system so we are not just testing the chip any more. In the case of high-speed components, the test equipment has not quite caught up with the component capability, delivering and collecting high-fidelity 200GHz electrical or optical signals that are calibrated right to the chip is a challenging task. The drivers that we build in products are integrated with the components to work together and deliver system performance. As a result, what we measure at component level in the lab differs from what we build and test at the module level on the production line. System problems are passed back down the line to align with component test data and then on to simulation data to inform design changes.

It may appear that joining the simulation and the real world is ‘simply’ a case of fitting. This artform takes real or artificial intelligence to adjust hundreds of simulation parameters to agree with the measured data and inform adjustments to hundreds of process parameters. However, different groups in the business use different parameters for materials. E.g. growers often define materials by their strain and SE peak (but in a defined calibration composite structure), since the measurement tools are X-Ray and PL mapper. Simulation often uses just material composition (x,y) since bandgap and strain are then calculated. Simulation is often based on carrier density, whilst experimental data is driven by current. Whilst converting between the two is supposed-ly simple, the reality is that multiple data are needed e.g. light-current and relative intensity noise (RIN) spectra are both needed in order to have sufficient degrees of freedom. In addition the device that is actually fabricated can differ significantly from the one in the model. Perfect shaped structures with abrupt interfaces are often modelled but non-uniform shapes with contamination, dopant migration, material alloying, unwanted charge are realised. Structural investigation (SEM, TEM, SIMS) is used to understand the differences, along with specific opto-electrical test structures tailored to de-embedding parameters.

V. Matching Simulation To Test Is Not The End

Journals are willing to accept world beating results on their merit alone, but customers are not. There is now a question of reliability. Many devices across many wafers are over-driven to see how they die. The failure modes are investigated at great length and related back to process or design. Once understood we can drive activation energies and acceleration parameters, to derive the failure in time rate and device lifetime for normal operation. If there are any problems relating to design, for instance; the operating current density, junction temperature or strain then a re-design is required. If we have been so bold as to employ new materials, then we may find that further growth studies are needed and we begin the entire R&D cycle again.

Assuming that all is well, we have made a device that meets all the product specifications, exceeds the yield cost model and is beating any competing technology offered by competitors. The company makes money, technology moves forward re-invests in R&D, we keep our jobs. However we are given the enviable task of improving the device again by doubling the speed, power, efficiency or suchlike, and so the cycle continues.

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