HETEROGENEOUS INTEGRATION ROADMAP

2020 Edition

Chapter 14: Modeling and Simulation

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Chapter 14: Modeling and Simulation

1. Executive Summary

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The 2020 edition of the HIR modeling and simulation chapter contains minor updates to all sections detailed in the 2019 edition, as well as new sections on materials characterization and systems-level modeling. Design and Modeling and Simulation (M&S) tools are key enabling technologies for Heterogeneous Integrated Electronic Systems that will support product development across the chip-package-board-system domains. This chapter details the key challenges and potential solutions over 5-, 10-, and 15-year horizons, and detail how these tools will support the knowledge base for heterogeneous integrated electronic systems as detailed in figure 1.

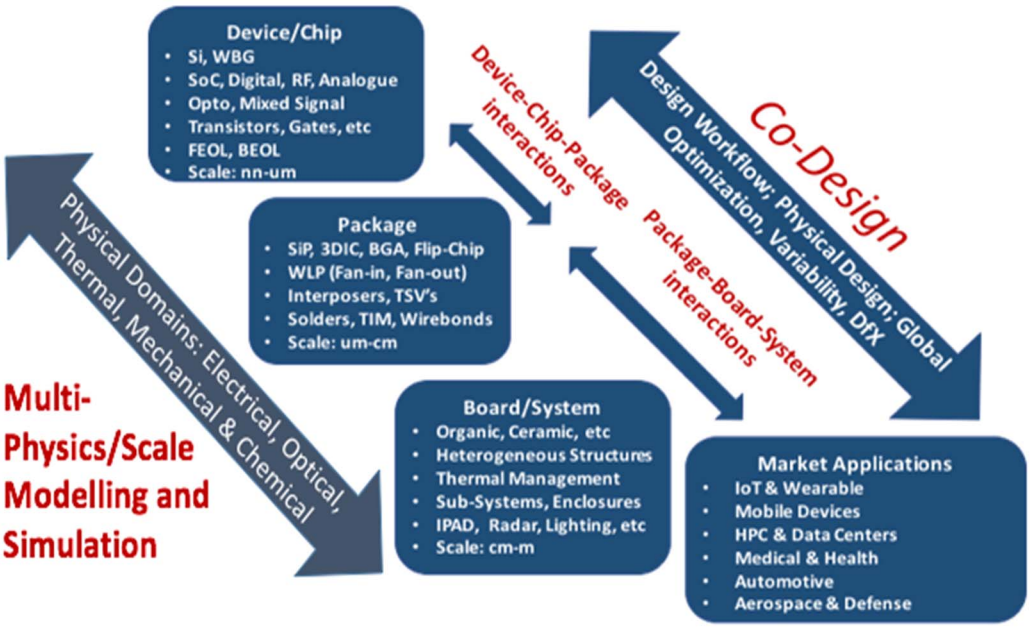

Figure 1: Supporting the Knowledge Base for Heterogeneous Integration

Analysis using M&S tools today can generally be classified as being single physics (electrical, optical, thermal, mechanical, chemical), single domain (Die, Package or Board/System), with a few design points investigated. The future will require multi-physics/scale capabilities, design collaboration (die-package-board/system), and system aware analysis. The results from modeling and simulation tools will also be required to support the development of both process and assembly design kits (PDKs and ADKs).

For example, influences from other physics is assumed in a crude manner (e.g., package thermo-mechanical stress generally assumes a constant temperature profile, where in reality, the die electro-thermal behavior and hotspots are transient; and detailed board behavior and its constraints are generally ignored). For integrated heterogeneous systems, such assumptions will become invalid.

2. Scope

The Modeling and Simulation TWG considers challenges and potential solutions for modeling and simulation tools in the following areas:

1. Electrical Analysis
2. Thermo-Mechanical Analysis
3. Mechanical and Multi-Physics Analysis
4. Materials and Interface Characterization
5. Molecular Modeling
6. Systems-Level Modeling
7. Reliability and Prognostics

In addition to the taxonomy of the modeling and simulation categories listed above, the chapter also focus on articulating the key metrics in a quantitative (wherever possible) and qualitative manner.

As well as defining the challenges and potential solutions in each of the domains, the need to undertake co-design to model and predict key physical interactions through the use of multi-physics/scale modeling capabilities will become critical for supporting product development across the chip-package-board-system domains. These challenges will be captured for each of the domains and related to the key device-, packaging-, and system-level challenges defined by the other chapters in this roadmap and in particular, Chapter 13 on Co-Design.

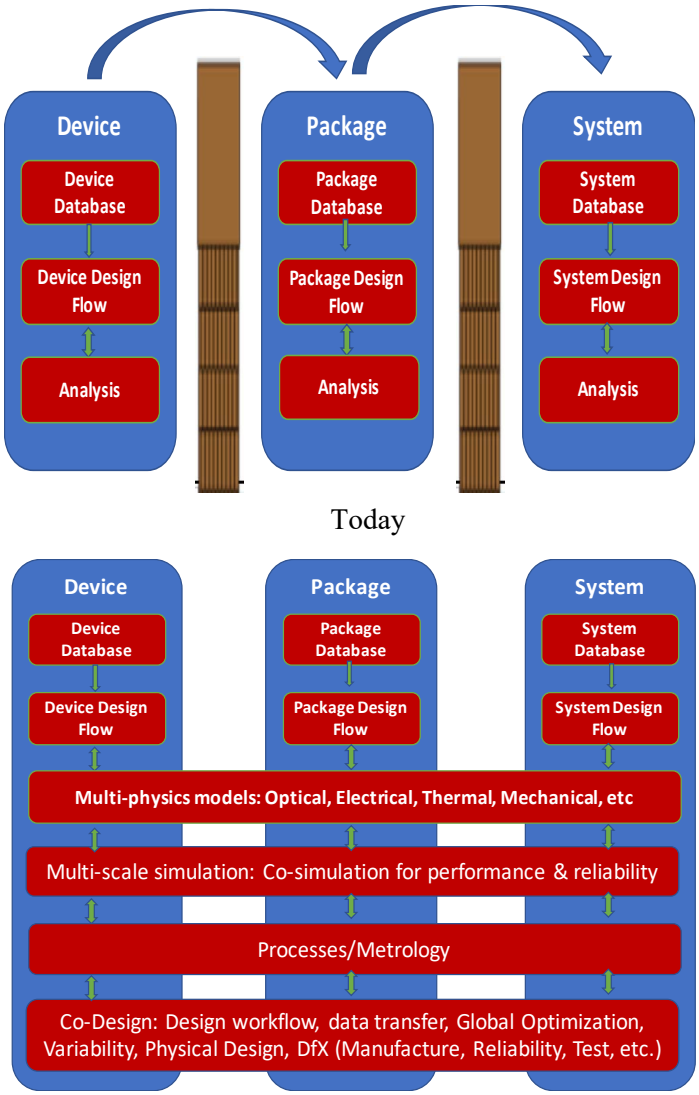

Figure 2: Moving towards a new M&S paradigm

3. State of the Art, Difficult Challenges, Potential Solutions

Modeling and simulation tools can be defined by different levels of abstraction, from circuit simulators such as SPICE to computationally complex models using molecular dynamics, finite elements, and computational fluid dynamics. Traditionally, thermal and mechanical analysis was undertaken by systems designers who would then pass on the requirements/constraints to package designers. Chip designers mainly focused on electrical analysis, which, today, for highly detailed system-on-chip designs is very challenging. But chip design can no longer avoid issues related to thermal and mechanical stress, particularly for 2.5D/3D heterogeneous packages. Multi-physics interactions must now be taken into account. Hence a paradigm shift in design tools is required that, together with electrical analysis, addresses both thermal and mechanical issues in the chip design flow. Multi-scale modeling must address the need for modeling chip-interactions at the nm scale (e.g. transistors), package interactions at µm-mm scale (e.g. TSV, Microbumps), and mm-m scale for systems (heat sinks, PCBs, etc). A mesh-based model, such as

finite element or computational fluid dynamics, cannot be used to address the multi-physics interactions spanning these scales. This is also the case in the time domain, where key electrical effects can take place at ns scales, whereas thermal and mechanical issues can take seconds or even years (in the case of reliability) to appear. To address the issue of dimension and time scaling, modeling techniques based on sub-modeling, compact models or response surface models is required.

For heterogeneous integrated systems, what level of model abstraction is appropriate, and how we exchange data effectively between these, is a key challenge. Figure 3 details examples of models of different levels of abstraction that are used for optical systems.

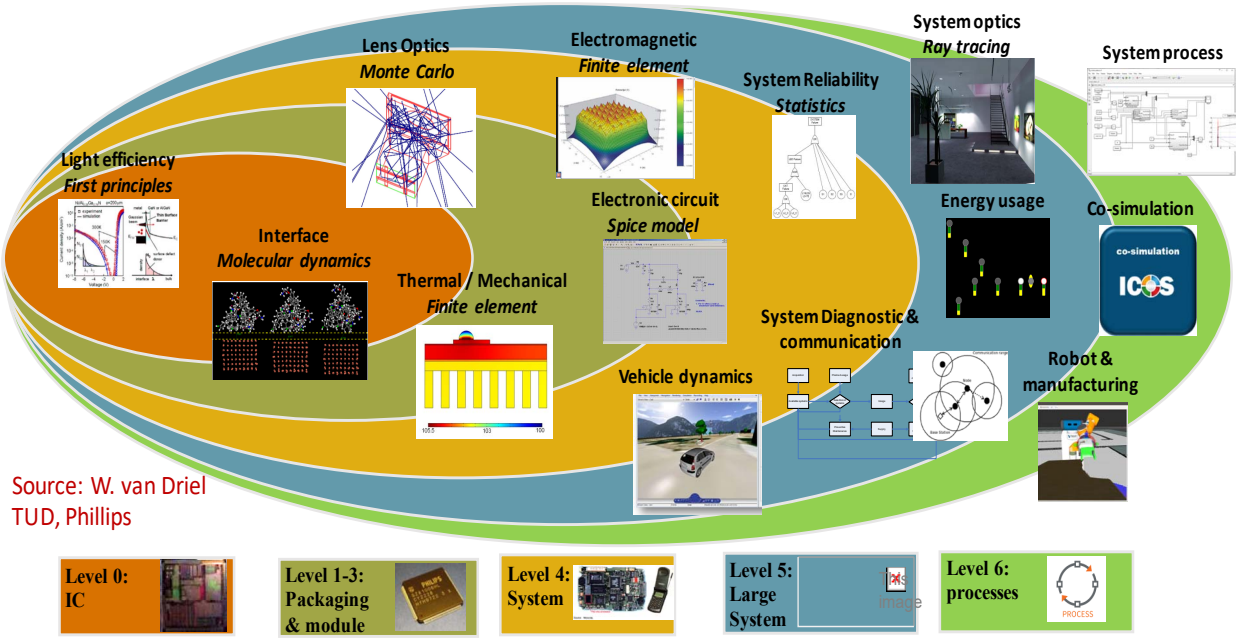

Figure 3: Modeling and simulation landscape for photonics

Simulating the behavior of heterogeneous integrated products will require co-design, co-simulation, and multi-physics toolsets that can accurately predict physical phenomena across the length scales. In the future, there will be advances in measurement equipment and data from sensors that will require the use of big data analytics and machine learning, as well as physics-based models to support co-design and the knowledge base for heterogeneous integration.

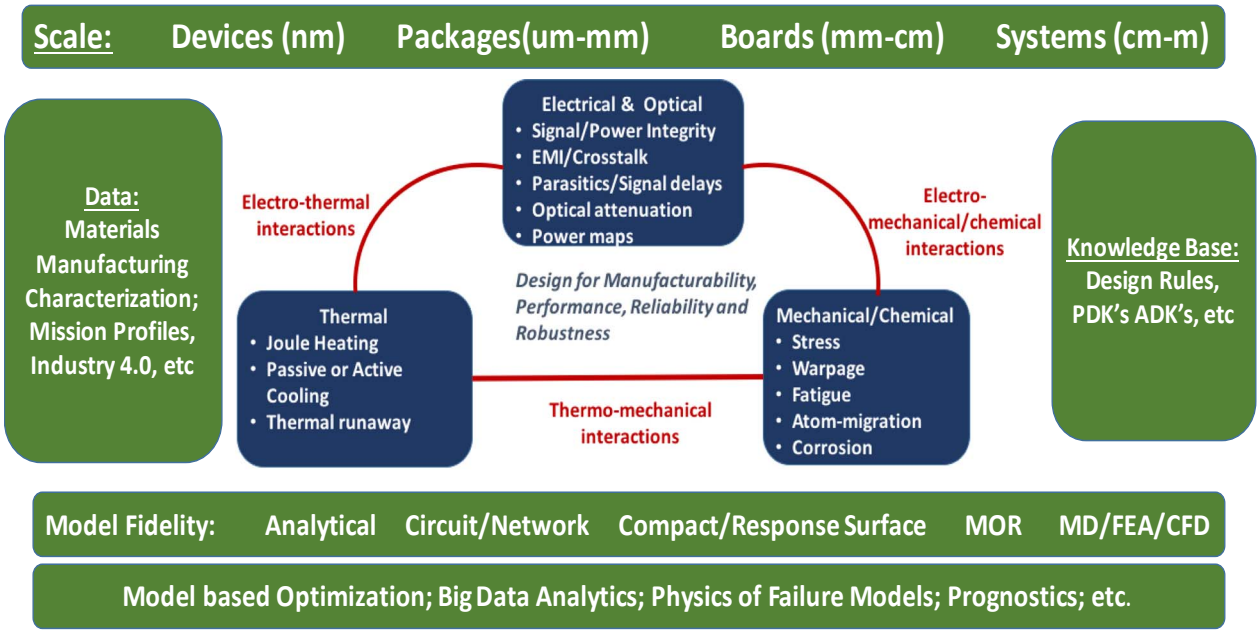

Figure 4: Modeling across the length scales

While Moore's Law economics has come to an end, scaling to advance nodes continues with EUV processes and 3D FinFET design. Companies presented 3nm FinFET technologies at IEDM in December 2018, projected for the 2022-2023 timeframe. Today Chip-Package Interaction (CPI) involves trade-offs between ILD and the top metal layer on the chip, with UBM solder/copper pillar and chip-package design. Looking ahead a few years, with FinFET and FinFET GAA at the 3nm node and beyond, there will be the additional dimension of complexity with transistor self-heating that must be taken into account. Additional consideration will be differing requirements for different markets – Mobile (consumer smartphones), Data Centers, Mobile Networks, and Automotive.

The following sections detail the current state of the art and identify key challenges that need to be overcome.

3.1 Electrical Analysis

Current State of the Art and Requirements/Challenges

To understand the challenges of electrical design of electronic systems with heterogeneous integration, it is instructive to evaluate the current methodology, analysis capability, and limitations for non-heterogeneous, individually packaged components. The electrical analysis focus for the electronics packaging engineer is signal integrity, power integrity, and electromagnetic radiation and susceptibility. The multi-physics may include electrical and thermal interaction for digital or analog circuits and designs, or physical shape-changing in some RF applications.

The current state-of-the-art reflects the hierarchy of component design, the physical scale of the component under evaluation, the spatial separation of components, and the electrical parameters of primary concern. For example, a silicon die includes billions of interconnect segments on a micrometer-level scale, dimensions less than a wavelength, bump pitches near 100 micrometers, and heat dissipation of tens of watts per square centimeter. In contrast, a printed circuit board has thousands of interconnects on a 100-micrometer scale, connector pitches near 1 millimeter, multiple bits stored on the interconnect, and heat dissipation is joule heating of milliwatts per square centimeter.

Currently, the details of the electrical analysis are customized for each component. The signaling interconnect analysis is dominated by resistive loss, crosstalk, and signal delay at the semiconductor level. However, at the printed circuit board level, the loss due to the dielectric loss tangent and copper roughness becomes significant. At the semiconductor level, a sub-micron scale is needed for extraction, while for the printed circuit board, the scale is much larger. However, nanometer-level roughness is needed for surface impedance formulations in a printed circuit board. The methodology for the extraction of these details is facilitated by an independent analysis of each level of component, and by the creation of specifications and budgets to communicate with the adjacent levels. Therefore, the electrical analysis can be performed one component level at a time, and co-design and co-analysis can include the semiconductor die details in the package analysis for the purposes of power distribution analysis, for example.

For the semiconductor die, the physical structures are small compared to the wavelength; static solvers that solve the electric fields and magnetic fields separately are desired. These solvers are fast computationally and rapidly extract lumped element models for complex 3D packages. Most commercial static simulators can generate SPICE equivalent circuit models, which can then be used in chip-package circuit SPICE simulators.

For printed circuit boards, where the structures are large compared to the wavelength, high-frequency analysis that includes the coupling of the electric field and magnetic field are required. Such analysis requires the use of full-wave 3D field simulators that solve the wave equation derived from Maxwell's Equations. High-frequency behavior such as transmission line, skin depth, and radiation effects are captured in these simulations. Most commercial tools can export frequency-dependent s-parameter models for the interconnects. These can then be used in SPICE simulators, which can handle full-wave s-parameters in both time and frequency domains by creating compact models based on pole-zero and/or state-space modeling. For high-speed channels with serial components, however, simulators with a behavioral representation of channel equalizers at the transmitter and receiver and statistical analysis of the noise and jitter components are also included, which traditional SPICE cannot practically include.

Today, not only are the tools independent for each component level, the time of the design and analysis likely does not overlap. The individual (largely independent) tools and methodology for each component level allow a system design to depend on components that are being designed on very different schedules by different teams for non-heterogeneous designs. For a logic semiconductor component, the design schedule from concept to logic entry to physical design to tape-out is much longer than a package design schedule, and the packaged semiconductor is likely completed before the printed circuit board design. The silicon design team would be redeployed before the printed circuit board design begins and even if co-design could be done, it would at best give a more accurate analysis of the final signal or voltage waveforms with an optimized PCB; hence, it would not improve the semiconductor design or

enable an optimization of the design across the package hierarchy since the semiconductor component is already being manufactured. A broad segmented supply chain has developed to support this model of design.

Currently, the state-of-the-art heterogeneous integration electrical analysis tends to depend on designs that have multiple components by one company or group where schedules and design details can be shared and coordinated. Procured components, such as stacked memory, have detailed specifications to ensure proper operation when integrated with other components designed by other teams on a later schedule [1].

To fully exploit the performance capability of heterogenous integration in future systems, modeling, simulation, and analysis of the electrical operation and interaction of the closely placed components is needed. This can be co-design, so a team of designers can optimize a design with multiple semiconductor components and the packaging that contains them. This will include co-analysis to enable the simulation of the electrical behavior of this design. The co-analysis can also be used to increase the simulation accuracy of a completed design.

The co-design with co-simulation is critical for first-time-right designs and optimizing the performance, specifically the power-performance and cost-performance of the system under design. The co-analysis of the completed design is critical for analyzing the important performance parameters of the completed design. It is also useful for verification, characterization, and debugging of the final hardware. In the past, physical probes with time-domain or frequency-domain measurements could be done on individual components at the printed circuit board level; with heterogeneous integration, one will depend on internal registers for observation and then perform a simulation to understand the electrical or thermal behavior in the event that unexpected system operation is encountered. This is an important need case for accurate co-analysis.

This co-design, co-simulation methodology will benefit greatly from 1) standardization of interface files for tools, 2) sharing of physical geometry description, and 3) standardization of specification of compliance of channels. This implies a specification of the requirements of the signal into the receiver of a channel and how jitter components are calculated and summed on the channel.

- The standardization of interface files could range from a design kit for a set of devices that belong to a closed ecosystem of like products to truly open standards enabling innovation by integrating a broad range of products into a design.
- The closed ecosystem of like products exists today in early forms, and the truly open standard should be a long-term industry objective. Sharing geometrical description of components that the designer considers proprietary is currently done in a limited way with encrypted files suitable for 3D electromagnetic solvers. Extending this capability of securely sharing physical data to integrate the geometric extraction across multiple components will be needed to enable future multi-physics co-analysis, of which a simple example is analyzing the impact of temperature excursion on one component impacting the metal resistance in another component without divulging the details of the proprietary design.
- The standardization of the specification of compliance can start with standards that exist today for channels such as PCIe or SAS. Future standardization can include the previous two points of interface files and physical geometrical information, but ultimately, the various tolerances that make up a channel also need to be reflected in the channel analysis. These include manufacturing tolerances of physical dimensions, circuit tolerances to voltage and temperature, and variations caused by assembly tolerances.

The above has addressed the passive channel and touched on the behavioral circuits for the transmitter, receiver, and equalization circuits for a digital serial high-speed channel. Successful adoption of heterogeneous integration will depend on combining functions such as RF, analog/mixed signal, DSP, and EM to the digital channels. These analyses are performed today using a broad range of simulation tools. Disparate chip functions require different simulation technologies resulting in a range of simulation tools distinct from each other. For example, frequency-domain simulators are suitable for RF applications, but time-domain simulators are used for digital applications. The system design process will provide predictions of package behavior and interconnect parasitics across levels of packaging; simulating these functions together will allow modeling the interaction between components. This is a challenge for simulation tools in terms of convergence and solution times. Currently, designs budget noise and jitter impact and isolate sensitive components. The drawback to the current approach is two-fold: the design will take more physical volume to isolate components and more modeling and simulation effort to confirm isolation than what may be required. In addition, when functional issues are discovered with hardware operation, simulation is of limited use in the diagnosis of unexpected electrical behavior.

Potential Solutions

Future co-design and co-simulation need to address multiple physical components, as discussed above. The scale of features both in size and number in a semiconductor device, compared to a printed circuit board, highlight the challenge. In a five-year horizon, the component providers will extend their existing methodology to incorporate the details of the surrounding components. For example, a designer of an integrated package will expect more detail on the semiconductor devices being assembled, whether they are digital, RF, or mixed signal. Behavioral models of switching circuits, signal and power distribution networks, and noise susceptibility are needed for robust design. As the integration capability advances with embedded devices, stacking and TSV interconnection of devices, as well as increasingly sophisticated interposer and redistribution wiring technology between devices, the design and simulation tools and methodology need to stay in step.

During the five-year horizon, specifications will be developed, and efforts will be made to further define the tools and methodology for analysis for companies working cooperatively to specific standards. In the five- to ten-year period, the methodology could develop into sharing of designs more broadly through the use of sophisticated standards or even encrypted physical features and descriptions along with industry agreement on how to incorporate them into the tools. The success of this effort depends on how companies align themselves as integrated component designers and suppliers or distributed independent component suppliers to a final solution provider. In the 15-year outlook, the design tools and electrical analysis tools will reflect how the industry has developed, and in any case will need to seamlessly integrate the components as this part of the industry has matured, and differentiation may come from cost and the ability to integrate capability to meet the needs at that time.

Integration of electrical and thermal analysis will progress during the near term. Electrical-thermal co-simulation needs to be able to handle increasingly detailed simulation on a single package or component level and this capability needs to be further developed and extended to multiple-component analysis with diverse functions such as RF and digital [2]. Currently, commercial software extraction and analysis tools are available to analyze the interaction of the electrical and thermal response in a printed circuit board, package, or semiconductor device. Extending this analysis to multiple levels of packaging and circuits, and modeling the interaction between multiple devices, will progress along with the design progression described above [3]. In the mid-term of five to ten years, the industry needs to drive towards a methodology of thermal and electrical analysis across devices where details can be specified and shared, say in a consortium. In the longer term, the methodology needs to accept devices with details that are proprietary and not restrained to closed design communities to exploit the potential capability of heterogeneous integration.

Power integrity analysis needs to be increasingly integrated into the signal integrity analysis. Power and signal integrity traditionally have a different physical boundary for electrical behavior, creating the need for models and extraction of different physical dimensions. In addition, simulation times can be different for power analysis and signal analysis. A signal integrity simulation needs to resolve picosecond time steps during signal rise- and fall-times while analyzing millions of signal pulses. A power integrity simulation may be of most interest in the tens of megahertz to gigahertz range for a package design. The noise in the power distribution created by switching circuits of adjacent components needs to be included in the analysis, which increases the physical size of the geometry being analyzed compared to a typical analysis today. Crosstalk between adjacent signals in the densely wired packaging needs to be included in the analysis, and likely isolated in the design. These include large-swing digital signals and more sensitive RF circuits, which may not be so closely placed in a typical design today.

Compact models will be an important part of this timeline as an efficient way to represent the features of the components that comprise the design. The compact models must:

- enable the co-analysis of multiple semiconductor devices, the packaging, and the printed circuit board;
- handle the range of physical dimensions from semiconductor devices to printed circuit boards;
- include the electrical parameters for signal integrity, power integrity, radiation, and susceptibility;
- have the models and parameters to perform electrical-thermal co-analysis.

A roadmap for development of compact models needs to be developed and coordinated among the disciplines. The four areas are currently at different levels of development, which needs to continue in light of the long-term need to have the models compatible with each other and with the technology being developed.

The development of co-design and co-analysis methodologies along with the models to facilitate the methodologies creates the opportunity to apply machine learning and deep data analysis to the designs. Deep data techniques will enable design space exploration to accelerate the capability of the designs. A possible timeline would be to use deep data techniques to improve approximation techniques for signal integrity, power integrity, or thermal response in the next five years across the design space of individual components, and in the middle term of five to

ten years expand the techniques to approximate response of co-analysis techniques. Independently, the ability to analyze across multiple components can be developed. In the long term, combining the ability to explore the design space for co-analysis and multiple components simultaneously is a goal.

For machine learning techniques, in the near-term learning from existing designs to quickly and optimally designing subsequent design is a possibility. Progress is also being made in extrapolation techniques to predict bit-error rates from machine-learned simulation responses and expanding design rule checking to identify physical features that are unacceptable for electrical performance. In the medium-term time line, extending machine learning techniques to include more process and design parameters is essential to exploiting the potential capability. The uncertainty analysis of these designs with a sufficient number of parameters should be a priority. In the long term of more than ten years, machine learning has the potential to be disruptive in how designs are performed and analyzed.

System performance metrics are creating the necessity to invest in tools and methodology for electrical modeling and simulation as critical hurdles are encountered. Examples at two extremes of current channel design are long-reach channels utilizing PAM-4 signaling and dielet interconnection in a package with dense, wide parallel buses.

For the long-reach channels, the length of the channel, high density of wiring, and high data-rate create a focus on crosstalk to result in a signal to crosstalk ratio sufficiently large for successful data transmission. The resulting physical design can be guided by electrical constraints in a more systematic manner, possibly using machine learning techniques to guide engineering implementation. On the coding side of long-reach channels, techniques such as forward error correction (FEC) add unacceptable latency to the channels. Minimizing the latency is actively being pursued, and integrated coding-aware simulation could optimize the pre-route definition of the channels, assist in verification of the design before tape-out, and aid in characterization and diagnostics during system run time.

To optimize dielet interconnection within a package, power delivery is a top concern. The modeling and simulation integrated into the co-design tools for placement of dielet power and signal bumps and integration of decoupling capacitors while minimizing the power per bit needed to meet data rate objectives are system-level performance needs guiding the capability of modeling and simulation tools. In addition, the simulation capability of dielet wiring that takes the system performance constraints and is able to predict transient currents and spatial gradients of voltage are factors that thermal tools and reliability models can use to optimize the placement and life of the components.

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[2] Modeling, Simulation and Design Tools, A chapter of the 2017 iNEMI Roadmap.
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3.2 Thermomechanical Modeling

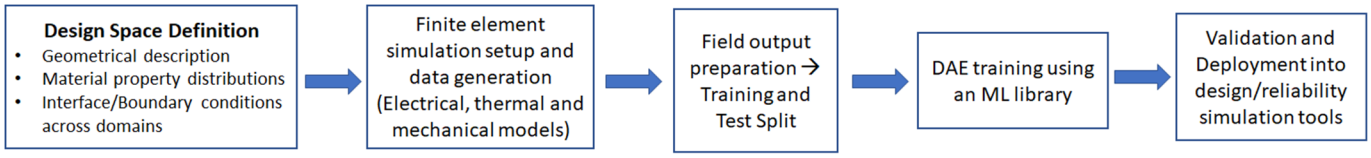
Current State of the Art and Challenges: The vast majority of thermal/thermomechanical design rules in electronic design and packaging are based on finite element method (FEM) based simulations post electronic design [1]. Robust thermomechanical models are not present in the electronic design and reliability flows, thus necessitating significant margins from the designers. The power dissipation and power density in future 2D-3D packages is expected to increase, and the cross-talk between different functional components of IC packages will further aggravate the thermal management challenges. This will necessitate the development of multi-physics simulation tools with closely coupled thermal, mechanical, and electrical models to enable iterative simulations and robust design. Such coupled models that can enable comprehensive analysis and design in reduced time have not been developed. One of the challenges with existing tools is the ability to accurately predict temperature across the length scales. These tools should allow coupling between different scales, e.g., die to package and package to system, to consider the effect of design at one scale on the other. Furthermore, high heat flux components within packages requiring single- or two-phase liquid cooling pose further challenges in quantitative modeling of two-phase fluid flow and heat transfer – an area where simulation accuracy is still developing.

One powerful technique that has re-emerged in the past decade for modeling the thermal behavior of large electronic systems is the use of reduced-order modeling through proper orthogonal decomposition (POD). POD enables scalability of accurate full-field thermal simulations (or measurements) from individual blocks to reconstruct large inhomogeneous domains and has been successfully applied by several groups from FinFET circuits [2], interconnects [3], and server racks [4] to IGBT and LED modules [5-7]. A natural extension here is to leverage developments in machine learning, combining them with physics-based thermo-mechanical models for high fidelity prediction of performance and design of these cooling technologies. Different types of machine learning models such as support vector regression, Gaussian process regression, or neural network could be applicable depending on the

application under consideration. POD combined with a machine learning framework, can be used as an equation-free approach for the modeling of nonlinear transient systems and can be applied to a wide range of applications.

Potential Solution: We discuss the needs and possible approaches for developing such next-gen modeling and simulation tools. FEM-based simulation tools for electronic design suffer from lack of multi-physics modeling capability, coupling across the scales, and maintaining high accuracy while making predictions in reduced time. Here we suggest a paradigm shift to better model, optimize and design for die- and package-level thermomechanical effects. The primary aim of this framework is to use a repository of finite element simulations packaged through a neural network engine and abstracted into usable design models. The following workflow is proposed to enable this early absorption of thermal and mechanical models into design tools:

- Definition of the design space and execution of FEM simulations with combinatorial and probabilistic input parameters spanning geometrical descriptions, material properties and interface/boundary conditions across domains.
- Training Data: Output FEM state distributions and fields (electric field, power density, temperature, stress, strain etc.). Training and validation using an artificial neural network with feedforward deep auto-encoders (DAE).
- Deployment of the validated DAEs generated to accurately predict the non-linear and statistical behavior of a design with minimum computational and setup overhead.



One example of such deployment in the thermal domain is by Zhang et al. [4] who apply machine learning to real-time thermal prediction/management and demonstrate improved accuracy, as well as significant runtime overhead reduction.

Importance of Accurate Materials Properties for Thermal Predictions: As HI takes shape, glass/Si-based interposer and 3D packages with stacked die will allow for integration of different functionalities with widely varying range of power dissipation in both space and time, also calling for simultaneous deployment of various thermal management solutions such as phase change materials, high conductivity anisotropic materials and direct liquid cooling. In addition, next-generation packages will need novel dielectrics, insulators and conducting materials. System-level simulation based on existing FEM techniques will get increasingly intractable while making thermomechanical estimates ever more important. We believe the path forward is to integrate first-principles material models (with specification of uncertainty) into multiphysics modeling tools to generate a comprehensive training set which are then put into machine learning frameworks to enable rapid design space definition, such as that shown in the workflow above.

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3.3 Mechanical and Multi-Physics

Current state of the art and challenges

Stress modeling of heterogeneous systems should contribute to the following: (1) design for reliability (stresses as inputs to reliability models); (2) design for yield (stress contribution to development of chip-package-system design rules); and (3) design for cost-effectiveness (identify lowest-cost designs and materials available to achieve reliability requirements).

For traditional packages, the material and mechanical design of the chip, package, and system had relatively large margins, since stresses were well below the material failure limits. Hence, stress modeling is used only after a failure has occurred. However, for advanced packages and heterogeneous systems, many factors (cost reduction, new materials, form-factor reduction, etc) may drive the stresses to the limits. Hence, stress modeling should be considered at the early stages of design as a precursor to predicting reliability.

Stress modeling using finite element techniques has been reported widely, and a number of commercial finite element codes can be used to predict phenomena such as:

- Interconnect (solder joints, etc) stress;
- Board warpage;
- Full system to chip interactions;
- Stresses in through-silicon vias (TSV's).

At present, the majority of stress analysis performed is at the package or board level. Chip-package interaction has also been studied, but is becoming more important, and die designs now need to consider the stresses imposed on the die from the package. Simulations have also shown a significant effect of the system (mounting) situation on chip and interconnect stresses [1],[2]. Hence, there is a need for chip-package co-design in terms of package design on the subsequent stress states at the BEOL and FEOL of the die and the impact these will have on the performance of the die.

Modeling and simulation tools have the capability to simulate the mechanical behavior of a package which is subjected to a number of environmental conditions such as temperature, vibration, shock, etc. MCAD Tool vendors provide co-design capabilities that include thermo-mechanical analysis, including effects such as thermally induced stress, and sub-modeling techniques can be used to transfer results from the system (board) level domain to structures at the die level as detailed in figure 5. However, these capabilities do not generally have accurate models for critical failure modes that will be important in 3D heterogeneous systems. Also, there are weak linkages between these MCAD (finite element) tools and EDA tools for electrical analysis to support full chip-package-system co-design [3].

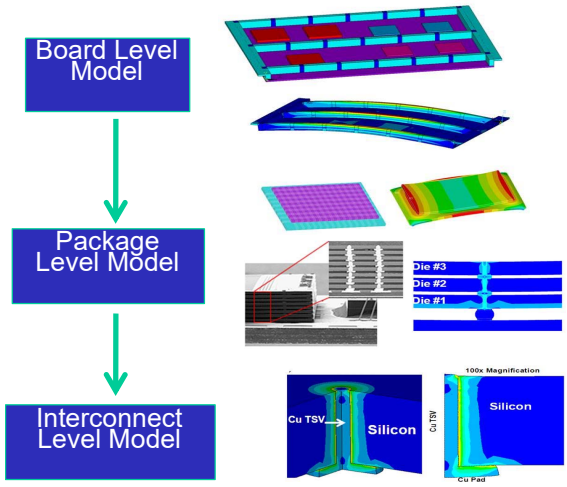

Figure 5: Mechanical chip-package-board design

Heterogeneous systems combine different functions together with RF, analog/mixed signal, digital, DPS and EM. When the power is turned on for an electronic device, due to Joule heating, hot spots and uneven temperatures will arise in the system. Furthermore, different materials, from chip to package to board level, will experience different thermal expansion. Therefore, the temperature gradient and thermal mismatch among different materials will generate thermal stress, which is the root cause of many failures in electronic devices.

Most of the mechanical simulation focuses on the thermal stress due to thermal mismatch only (isothermal condition). The effect of temperature gradient in transient or steady state is not taken into consideration. Moreover,

moisture absorption/desorption will also induce additional mechanical stress. For moisture-sensitive materials [5], such as polymeric materials, swelling will occur during moisture absorption, and contraction will occur during desorption. In this way, hygroscopic stress is induced. Additionally, during reflow, internal high vapor pressure will also be generated in addition to thermal stress and hygroscopic stress.

Electromigration, a critical reliability issues in electronic devices, is an enhanced mass transport process in the current-carrying metal induced by the driving force (electron wind) generated by an electric field [4,5]. The well-known Blech's theory on electromigration was developed more than 40 years ago, in which the electron wind flux is entirely balanced by the stress-induced counter flux at steady-state condition (see Fig. 6 (a)). The maximum stress that the metal line can withstand is used as the threshold of electromigration failure. Therefore, it has long been perceived that electromigration is due to mechanical failure. However, such an over-simplified stress-based failure threshold has several flaws. First, Blech's threshold condition is obtained based on the steady-state solution, but most of electromigration observed in experiments occurs before reaching steady state. Secondly, it has been generally recognized that while electromigration is induced by the electron wind force due to the high current density, mechanical stress gradient is not the only counter-force at work. The atomic transport during electromigration is influenced by a combination of several interacting driving forces (see Fig. 6(b)). These forces result from different physical causes, such as the gradients of atom concentration, electron wind, temperature gradient, and mechanical stress gradient. For the electromigration to be analyzed, self-diffusion, thermal migration, and mechanical stress migration must be coupled with electromigration for an accurate prediction.

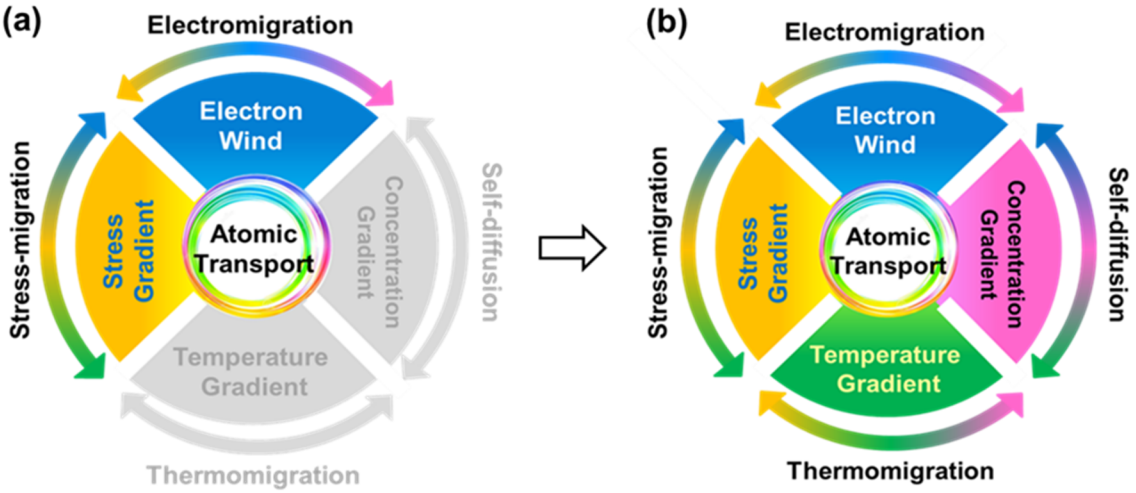

Fig. 6. Interrelations among electromigration, thermo-migration, self-diffusion, and stress-induced migration.[6]

In past decades, there are many research results on the formulation and solution of such a coupled physics problem for electromigration; however, inconsistent and incomplete solutions appear in literature, as summarized in Table 1. Recently, a newly developed model by Cui et al., [7,8], which fully couples those physical fields in a self-consistent and complete way, proposed a concentration-based failure criterion. That might be a more comprehensive criterion rather than the stress-based criterion, as electromigration is eventually determined by the void growth (circuit open) or hillock formation (circuit short) that is characterized by the vacancy concentration, regardless of the magnitude of mechanical stress. The implementation of such a multi-physics model has been completed with ANSYS [8].

The accurate simulation and modeling of electromigration are still under development. The coupling relationship between mechanical stress and concentration is an unsolved problem that can seriously affect the accuracy of electromigration modeling. Besides, a reliable model for mean-time-to-failure (MTTF) of interconnect based on multi-physics is required. Although the well-known Black's equation provides a useful empirical model for the prediction of electromigration failure, it does not allow a thorough understanding of the underlying physics related to the electromigration behavior. Tu et al. [9] recently tried to use entropy production to build up a unified model of MTTF, which might be a potential direction to improve Black's equation. Nevertheless, a more sophisticated physically-based MTTF model is required. For the nano-scale interconnects used in CMOS technology, electromigration strongly depends on microstructure, bonding strength, and interface material structure. The traditional FEM-based modeling is no longer satisfied with the requirement of S&M for electromigration. It is inevitable that the nano-scale modeling approach is needed to accurately predict electromigration failure.

Table 1. Summary of important physical models in the literature [6]

Physical models	Flux, self-diffusion	Flux, stress-migration	Sink/source term	Constraint condition	Stress equilibrium	EM strain
Shatzkes and Lloyd (1986)	✓	✗	✗	N/A	N/A	N/A
Kirchheim *et al.* (1992)	✗	✓	✓	✗	✗	✗
Korhonen *et al.* (1993)	✗	✓	✓	✗	✗	✗
Clement and Thompson (1995)	✗	✓	✓	✗	✗	✗
Suo *et al.* (2003, 2014)	✗	✓	✓	✗	✗	✗
Sarychev *et al.* (2000)	✓	✓	✓	N/A	✓	✗
Sukharev *et al.* (2004, 2007)	✓	✓	✓	✓	✗	✗
Maniatty *et al.* (2016)	✓	✓	✓	✗	✓	✓
Cui *et al.* (2019)	✓	✓	✓	✓	✓	✓

In addition, the novel interconnects and structural components in heterogeneous integration (HI), such as micro-bumps/pillars, hybrid bonding, RDL and TSV, can have distinct electromigration characteristics due to the parallel network configuration, where the standard weakest-link approximation used to evaluate electromigration lifetime would not be applicable and require new electromigration criteria for network systems. For the high-density RDLs used in fan-out (FO) packaging, the current density is approaching 5.4 $\times 10^5$ A/cm^2 to 6.0 $\times 10^6$ A/cm^2 when the Cu RDL is downsized to 1 µm and 0.3 µm feature size. [10,11] Not surprisingly, electromigration inevitably becomes a big concern for application of RDL in FO packaging. For a microbump of 10 µm in diameter, if there is a temperature difference of only 1°C across it, the temperature gradient is 1000°C/cm. That can cause unexpected electromigration and thermomigration failure. Furthermore, the wide bandgap (WBG) semiconductors, represented by SiC and GaN, are promising candidates in high-power semiconductor devices. However, the high operating temperature (~350°C) for SiC-based power devices is a big challenge for the electromigration performance of interconnects in power devices; a robust, practical solution to reduce the rate of electromigration at high temperature is needed.

For a heterogeneous system, there are various loading conditions: thermal load (temperature gradient or temperature change), humidity load (relative humidity applied in ambient), mechanical load (such as shock or bend), electrical current, and radiation exposure (such as UV radiation) etc. Therefore, the modeling must be multi-physics, which will involve either one-way coupling [3], [8] or two-way coupling of the relevant physics. Figure 7 shows the physics domain involved in the multi-physics modeling for a heterogeneous system.

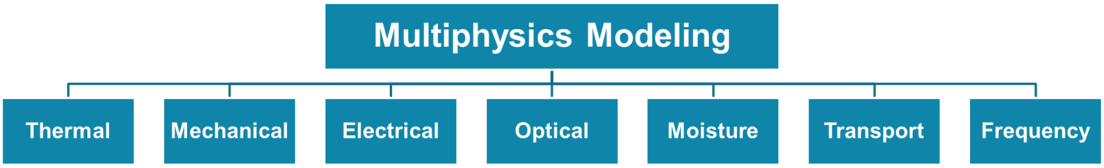

Figure 7 Multi-physics for a heterogeneous system

Currently available CMOS technology can already manufacture ICs with feature sizes down to a few nanometers. To assemble the IC into various packages to form heterogeneous systems, one has to deal with integration of geometric dimensions from nano to micron to macro-scales. Due to the huge scale difference, size effects will become essential. These size effects are often related to microstructures and their evolution, various gradient effects (such as chemical, electrical, thermal, and mechanical gradients), and surface effects. In addition, at the atomic level, it is virtually impossible to design a process with deterministic performance. At the macro-level, for design parameters

such as material/interface properties, geometric dimensions, process windows, and loading intensities, deviations represented by different statistical characteristics and magnitudes are inevitable. Figure 8 shows the evolution of microstructure of a copper metal line for different technology nodes.

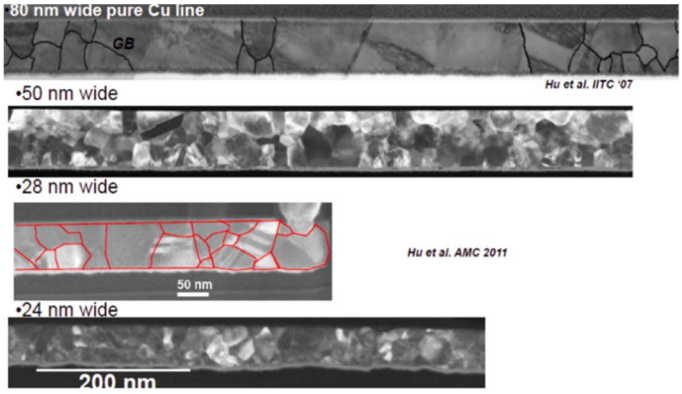

Fig. 8 Copper metal line scaling over the past generations of CMOS technology

Multi-scale modeling can include modeling at different levels, such as quantum mechanics, molecular dynamics, Monte Carlo methods and continuum mechanics (such as the finite element method). Each of the methods performs well for a particular level of accuracy. For example, density function methods provide a quantum-mechanical approach of electrons and nuclei, which is appropriate for processes such as chemical reactions and surface kinetics. Molecular dynamics offers many computational advantages over a full density functional calculation. Monte Carlo methods are especially useful for obtaining statistical information. Continuum methods provide a reduced description in terms of continuous fields for the coarse-grained evolution of the system.

Due to the strong interaction between multi-physics and multiscale, the complexity of modeling and data description, the large number and wide range of parameters under investigation, as well as the necessity to control and steer the simulation processes, accurate and efficient simulation of multi-physics and multi-scale systems are still not applicable. Commercial finite-element analysis tools all originated from the needs and knowledge of solving mechanical-related problems. Most emerging multi-physics software cannot yet deal with complicated engineering reality with strong nonlinear responses. Robust and easy-to-use multi-physics tools are still not available. Therefore, more effort should be spent on the development of sophisticated (multi-physics and multi-scale) models and efficient numerical algorithms.

Potential solutions

There is a need for new numerical techniques to solve stress, and possibly model-order reduction (MOR) can be one of the techniques. The challenge here is the highly non-linear behavior of materials (e.g. creep) which at present MOR methods have difficulty in solving.

Accurate materials data and characterization of a heterogeneous system is critical and hence greater links between metrology and stress and multi-physics modeling are important. Further work is required to transfer data from metrology into modeling tools (see figure 9), and there is a lack of consensus on accurate constitutive models used – for example, for non-linear materials such as solders.

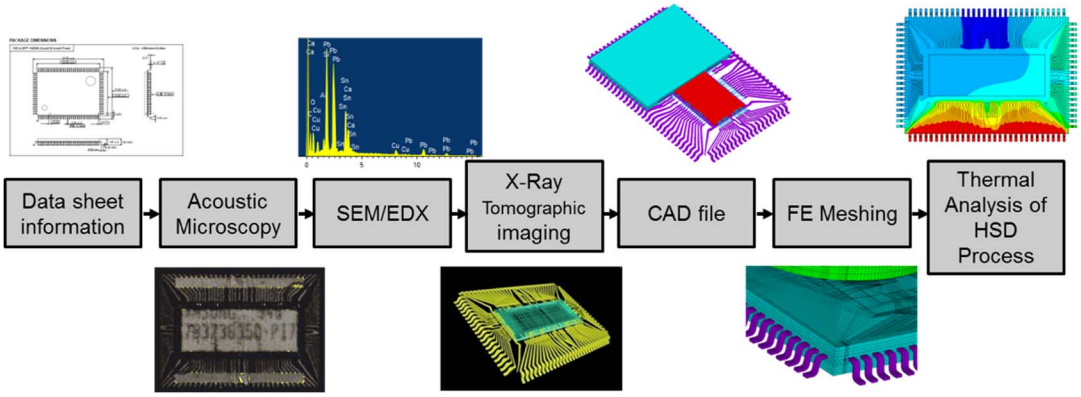

Fig 9. Integrating metrology with modeling

Stress and damage are dependent on multi-physics loads, and this needs to be addressed in modeling tools. Full co-simulation is required to predict electrical-thermal-chemical-mechanical performance across the length scales –

the chip-package-board-system. At present, we have point analysis tools, with designers undertaking stress analysis separately at the die, chip, package, and system levels. This needs to be improved.

EDA companies offer logical, physical, and electrical design systems, and linkages are provided to thermal analysis tools, but at present there is very little integration for stress analysis other than mapping thermal fields into a MCAD stress analysis tool. There is a need for much closer integration and for co-design of stress at device, package, board and system levels. It is clear that undertaking stress analysis for individual components without capturing system influences and constraints is not feasible for heterogeneous systems. The challenge is what level of abstraction is appropriate for models across the length scale. Again, model order reduction may provide opportunities here. Evolving multi-physics and multi-scale modeling tools are also required.

Importance of Accurate Material Constitutive Modeling and Testing Based Failure Criteria for Mechanical and Multi-Physics Predictions

Generally, processing, miniaturization and temperature-dependent non-linear material properties have to be used for almost all electronic materials. For example, the material behaviors of (nano-) porous sintering layered materials depend strongly on processing, in particular on the degree of porosity, which can be evaluated by both micro-cell modeling and miniaturized measurements [12,13]. Processing dependence effects span over a wide range from electronic polymers to metals and intermetallics [14]. For many interconnection technologies, properties of intermetallics are of major importance. Standard testing is rarely able to provide the data needed and, hence, experimental techniques like nano-indentation or local SEM/FIB based optical measurements are extremely important for simulation input.

Verification testing to derive failure modes and criteria is another important area for achieving simulation accuracy; this is a basic prerequisite for tools such as digital twins. In particular, very limited knowledge exists in the area of long-term fatigue failure of electronic interconnects. Known analytical models can dramatically overestimate e.g. the fatigue life of solder joints subjected to mission profile loads [15].

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3.4 Material and interface characterization

Current state of the art and challenges

All structural modeling is based on materials properties, the knowledge of which crucially influences the quality of the results according to the zeroth law of all computer programming a.k.a. "garbage in – garbage out". This also applies for multi-domain and multi-scale simulations required for heterogeneously integrated electronic systems, as outlined in the preceding sections. From an abstract point of view, such a system can be conceived as a 3D multi material – mostly layered – structure, where dissimilar materials are joined by different technological processes, forming a corresponding number of interfaces. [1] Thus the material and surface properties depend on their chemical composition, but also on the way they have been processed and loaded, as this determines the materials' structure, which in turn determines the materials properties. Due to the trend of ongoing miniaturization, size effects must be taken into account. Whenever a characteristic length inherent to a mechanism becomes comparable to a critical dimension of a specimen, size effects are to be expected. An example: hardening of metals during plastic deformation is noticeably different when diverging from bulk behavior already below 2 µm due to differences in dislocation motion, [2] a phenomenon which touches the structural scale. And plastic flow is very often used as a failure parameter for physics-of-failure based lifetime models. [3] Size effects of fundamental relevance are found for every physical domain (electrical, thermal, optical, mechanical), and these need to be addressed in package simulation.

Essentially all physical phenomena required for establishing a simulation model for heterogeneously integrated electronic systems, be it for molecular models for interface interactions or digital twin models on the system level, are based on a knowledge of process-structure-property correlations with respect to the respective physical domain – and finally quantity - in question. To establish such correlations represents the "holy grail" of materials science and will undoubtedly keep this community busy for decades to come. This includes surface characteristics, since they are especially important for properties such as thermal boundary resistance and adhesion effects with respect to performance and reliability. Thus, as for most packaging materials, the structure is not known (with few exceptions as e.g. for single crystalline semiconductors); they have to be characterized, since only on very rare occasions do manufacturers supply comprehensive and relevant data for simulation input.

As the packaging community is based on interdisciplinary science with immediate industrial application and value creation, those process structure property correlations are high on the agenda for simulation and characterization. And since seamless zooming over the length scales and across physical domains is becoming visible on the horizon, there are a lot of challenges to be addressed with respect to materials characterization.

Above all, all multi-scale and multi-field modeling paradigms (as highlighted in the previous sections) must be combined with *multi-scale characterization approaches* to validate the respective results on each scale and domain. On the material and bi-material interface level, this poses the following general challenges, which are all strongly interlinked:

(1) Fundamental understanding and process-structure-property correlations: On one hand, this includes in particular structural and surface properties, and feeds into the domain of fundamental understanding of materials and technologies. It also has to address the structural changes, as a function of processing parameters (also considering defects and contaminants, etc) and thus serves as validation for process modeling and all modeling involving structural information (ab-initio to meso-scale). Here, modern material analytics comes into play, in particular for studying in detail the physical effects at work (e.g. deformation and failure mechanisms during stress testing, surface species presence, thermal boundary effects, ballistic transport, phonon confinement, etc.).

(2) Constitutive model parameter generation: On the other hand, bulk and surface properties have to be evaluated to feed into (semi-)empirical models. This requires rapid, accurate and inexpensive methods for materials and interface testing as a function of processing parameters, size, and usually temperature as well as moisture (harsh environment) and in the time domain for transient response and aging. In order to furnish meaningful results, it is mandatory that test specimens have undergone the same processing (or load history after accelerated stress test) conditions as the real device would experience. This is a particular

challenge for interface properties and also the scientific domains where due to the complexity of the contemplated material system no fundamental theory is directly applicable (as is typical for e.g. back-end applications).

(3) As materials data in the age of digitization is a most valuable asset, and due to the huge and comprehensive effort to generate that data, it is a big question how to make that data available (e.g. to the community) and to assure their quality or confidentiality. This is especially important for system simulation tools as well as for validation of results within the community.

Potential Solutions

Currently, materials characterization is usually done on test specimens taken from the manufacturer and cut or milled to fit into the testing rig. The State of the Art (SoA) material and interface characterization comprises:

For the thermal domain SoA:

- Thermal conductivity, thermal diffusivity, thermal capacity and latent heat (for PCM), thermal boundary resistance (rarely) as function of temperature (rarely), effect of surface properties of adjacent materials, pressure, humidity and aging (rarely).

The challenges here lie with size effects (thin layers), thermal boundary resistance under realistic conditions [4,5,6] and surface characterization for surface species [7] (especially for nano-enhanced TIMs), testing equipment that allows measurement with low parasitic influences and at higher temperatures.

For the thermo-mechanical domain SoA:

- Young's modulus and CTE as a function of temperature;
- Polymers and composites: storage and loss modulus, linear viscoelasticity for the dry state, CTE, Tg, cure shrinkage and reaction kinetics, moisture swelling coefficient, fracture toughness at room temperature;
- Metals: elastic-plastic behavior (e.g. Ramberg-Osgood fit) as a function of temperature;
- Solders: viscoplastic behavior, mostly only including secondary creep as a function of stress and temperature;
- Sintered joints: elastic or elasto-plastic material properties, sometimes secondary creep;
- Laminates: Anisotropic linear elastic characterization (e.g. for organic boards);
- Bimaterial interfaces: linear elastic fracture mechanical data for critical crack growth in external mode-I loading.

The challenges here also lie with the inclusion of non-linear viscoelasticity and plastic deformation for polymers under humid conditions, elastic-plastic and viscoplastic behavior for thin metals films [8,9] and interconnect-size specimens including primary and secondary creep and their dependence on structural features (grain size, pore size, etc.) as a function of temperature and moisture as well as the change of these properties and degradation under accelerated stress testing conditions (vibration etc.). For the fracture mechanical characterization of interfaces [10,11,12] subcritical [13] mixed mode crack propagation, data is urgently required, at least for several key descriptors, and all this for some temperature and humidity boundary conditions as well as the inclusion of rate dependent and nonlinear effects. In order to keep measurement influences on the specimen to a minimum, specimen-centered approaches are adopted [14, 9]. This means: no clamping, no transfer, and measurement of the samples right from the production line. This may mean that measurement equipment has to be adapted or newly constructed to test such specimens. This is in particular inevitable for thin layers which cannot be characterized any more as freestanding samples. [15]

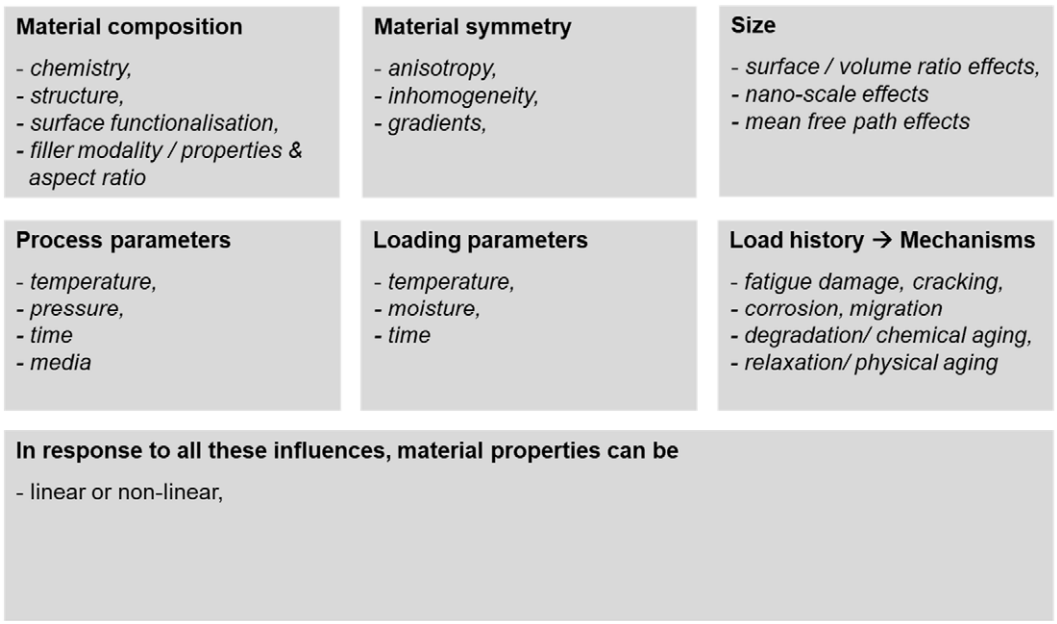

Figure 10: Material property dependencies on various influences. For engineering purposes, the materials have to be characterized to furnish relevant data for simulation input.

From the text and from figure 10 it is clear that the parameter space for characterization is rather large, the specimen preparation procedures rather resource demanding and the characterization equipment not always available everywhere. In order to be able to furnish the required material data within a short amount of time (orders of magnitude shorter that a PhD thesis), efforts have to be undertaken with respect to measurement equipment and procedures, meaningful accelerated stress testing paradigms, and specimen procurement in order to accelerate measurements, bring costs down and keep a working accuracy of the results along with a measurement protocol to allow traceability of the data.

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3.5 Molecular Modeling

Current state of the art and challenges

As feature sizes shrink and IO footprint densities increase, the materials issues must address a paradigm shift from bulk properties to direct inter-molecular or inter-atomic interactions. That is, it is realized that as the bulk-to-interface ratio shrinks, more importance must be placed on the molecular or atomistic interfacial properties, which are fundamentally different from the bulk properties. Molecular modeling [1,2] can be employed to help define the differences between the bulk and interfacial properties, and can identify how well specific molecular interfaces interact and how that interaction transforms to create failure. Molecular modeling can be employed at various stages in the life of the interface to inform the developer whether the risk in using a specific material is warranted, or to inform the reliability engineer which material/condition combination is at risk. For instance, the question of how the

interface structure evolves inherently must address several different questions: a) what is present at initial formation; b) what is present after all the processing steps are finished; c) what is present after low-level condition (stress/temperature) cycling; d) what is present after high-level condition (stress/temperature) cycling. Molecular modeling can be used to define structures present, from both chemical and physical transformations. In addition, molecular modeling allows a prediction of both the strength of a molecular interaction, and also how those interactions may transform under specific temperature, pressure and stress conditions. The basic goal in all molecular/atomistic modeling is the calculation of the energy changes and the accompanying transformations in the molecular structure that are responsible for the energy changes. The basic tenet is the belief that it is the evolving structures which describe the evolving interfacial properties.

All molecular modeling packages contain the constitutive equations which represent the atomic, molecular, and crystalline interactions. The packages are separated by the underlying assumptions made: a) quantum level (calculating the energies and resulting spatial interatomic characteristics resulting from atomic wavefunctions); b) molecular (calculating the molecular interactions from generalized atomic interactions found in force fields); and c) mesoscale (calculating higher size order interactions from parameterized molecular groups). The molecularly based mesoscale level is currently evolving; it is becoming popular to scale to higher length and time scales without the expense of larger computation power, which can be very useful when multi-interfaces are considered. An example of mesoscale interface failure is found in Figure 11, showing different levels of coupling into the cohesive side of an adhesive interface at failure, depending upon the type of deformation.

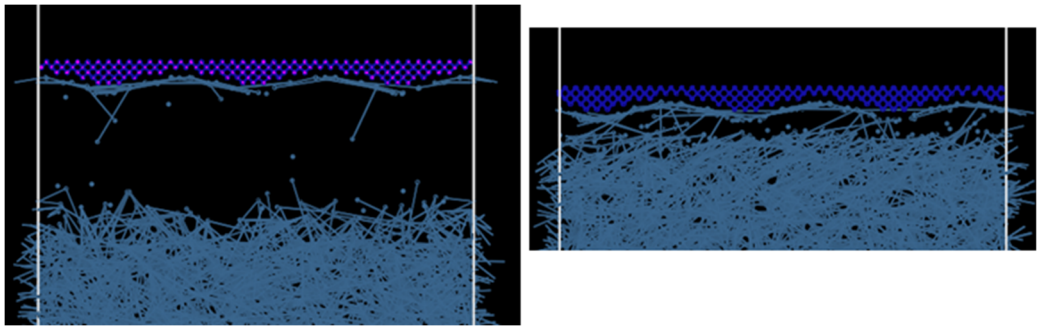

Figure 11. Mesoscale interfacial failure for a roughened (sawtooth) copper oxide-epoxy adhesive interface, for pure tensile deformation (left) and pure shear deformation (right)2,3 showing higher coupling into the cohesive side for the shear case.

Today, quantum level programs, on a practical level for industry needs, employ density functional theory (DFT), and are attractive because of faster solution speeds than traditional methods such as Hartree-Fock, and so can be used to quickly survey chemical changes at the interface, as well as survey interface bonding changes. The software should employ large enough basis sets and pseudopotentials in order to encompass the atomic elements of interest. For packaging, most software can handle most organic and silicone compounds; however, care must be taken that heavier transition metal elements (as well as lanthanides and actinides) are adequately handled. Although DFT methods have had issues with adequate representation of intermolecular interactions that affect accuracy, improvements are ongoing, and qualitative comparisons are still valid. In addition, interests in the stress response prediction on the electronic properties of the semiconductor (or other electronically active material such as ferro/piezo/pyroelectric materials) will require faster and more accurate solution methods. Of specific interest would be the mechanical-electrical coupling that would better predict how the semiconductor material responds to stresses inside the device or package, which could affect performance.

Molecular mechanics and dynamics (MM and MD) are available and readily employed today for most organic and silicone systems as parameterizations (forcefields). Forcefields are also available for more common metal-organic interfaces; although not all forcefields support all metals or their oxidized forms, the user can often look at the forcefield file to see if the specific atomistic parameterization is present. The forcefields provide the means to calculate the energetics of the interfacial systems by parameterizing basic physical dependencies of the interaction energies: the bond distance dependencies; the angle dependent energies; the torsional dependence; out-of-plane interactions; coupled interactions (such as bond-angle); non-bond energies (Van der Waals); and electrostatics.

How far structural transformations may progress (from crystalline and phase changes to nanovoid formation) really depends upon the size of the model; how large a physical feature size that can be modeled in a molecular model is directly related to the computer power, as most programs today are parallelized (or if not, are in the process of being parallelized).

Another area that is often promoted alongside molecular modeling software is property prediction techniques. They are roughly divided into statistical techniques and group contribution techniques. The statistical techniques like QSPR (Quantitative structure property relationships) and QSAR (Quantitative structure activity relationships) will generate a property equation of state for the user and then calculate the desired properties. They rely on data to develop the relationships between atomistic or molecular property descriptors (for example, simple ones are molecular weight, density, molar volume, functional group content, dipole moment) and the bulk property. There are many descriptors being developed today that make the techniques increasingly accurate, but these techniques are often hampered by lack of enough experimental data to generate a reliable relationship. Group contribution packages come with pre-embedded equation-of-state routines that calculate the property of interest for the user, based upon how much a certain atomistic property contributes to a bulk property. However, these equation techniques do not give the user a means to simulate how the material may transform, although they give quite specific information of what a material property may be under specific conditions. Future software will eventually develop transformation equations.

One of the most interesting emerging techniques today is the machine-learning neural network that will automatically develop the structure-property relationships based upon the molecular structure, and give the user the property of interest of the new/unknown material. This technique is also dependent upon experimental data to develop the properties, but unlike QSAR/QSPR does not require descriptors to develop the predictions.

Potential Solutions

The immediate requirements for molecular modeling to be practically applied in the packaging community is faster speed so that large-size molecular models can be implemented in less than a week. This is generally being addressed today by adoption of parallelized codes and adaptation within GPUs, which offer a speed-up over CPUs. Another practical need is expansion of techniques, some of which will be mentioned below.

Scientifically, there are many areas that need improvement. The quantum realm needs more pseudopotential development, which will be important especially for areas involving larger metals, such as the transition and lanthanide series (for example, for barrier metals and high-k materials). Other areas that need improvement and suffer from speed issues are phonon calculations so that more accurate thermal effects can be obtained. This is especially important for more specific thermal effect simulations. Expansion of techniques into direct radiation effects are needed, ranging from increased speed for quantum dynamic calculation to the calculation of radiation effects on the chemical that can be used to determine radiation hardening.

The molecular dynamics and mesoscale areas need better force fields for all metals and their oxidized forms (and other metal-based compounds such as chalgogenides), as well as interaction force fields with organics silicones and silicates. These modeling areas also need methods for force field auto- or semi-auto parameterization in order for the techniques to be readily available for new materials. The mesoscale levels have few forcefields available today, but are being developed. All force fields require inspection techniques for the user. An evolving area is that of reactive force fields. These types of force field could better handle bonding changes during an evolving failure path and phase transformations which will be important in metal failure. In addition, methods such as reactive potentials calculated "on-the-fly" are in development. Taken to the extreme, one vision is to be able to predict the product mixture (or a final state) from the reactant mixture (or initial state) which can become valuable when tuning industrial processes. Force field development will continue to be an ongoing effort and machine learning is becoming a significant focus.

On a practical level, molecular modeling needs simplified workflow development in which the engineer can simply pick and choose materials and material structures in design patterns, and the specific property can be automatically generated (adhesion, cohesion, diffusion, etc.). Simple workflows are usually available in commercially available molecular modeling codes today, but all techniques are not generally available. Also, workflows available still require knowledge of the molecular structure, so a certain amount of pre-model building is necessary and not ready for general pick-and-choose tactics. The pick-and-choose tactics for the engineer still need better definition – for instance, which structural variations can be generalized under a general particle force field, and which need specific definition and under what conditions. The mesoscale level may be a practical initial starting point from which to develop the structural assumptions, as the larger coarse-grained force-fields are themselves generalizations of the molecular grouping.

In addition, the link between the atomistic to molecular to mesoscale level needs further defining. On a wider scope, backward and forward scaling is needed between the microscale and molecular (atomic) levels, so that atomistic-molecular-mesoscale-microscale are readily bridged at-will. For instance, if the mesoscale level analysis finds that a certain interface is at risk, the modeler can zoom in to the molecular or atomistic level to define which

chemical structure is contributing (crystal, molecular or atomistic level). Length-scale bridging is an area that will not be immediately available, and is expected to be a longer-term issue (within the >10 year time frame).

In the future, it is envisioned that pattern recognition (and machine learning) will be used to simplify the structural choices for molecular modeling and become readily available for design and failure engineering, but will require extensive experimental data bases to develop the underlying structural assumptions and generalizations. For such data bases, cooperation between disciplines (both academic and industrial) is needed, especially to develop generalizations that link with the molecular structures with different interactions, and further with the properties of interest. Eventually, training the macroscale model could be done with neural nets, but most interestingly from the molecular scale, training the parameterization of the macroscale model from the molecular structure can be envisioned. However, how the neural net will treat issues of time domains (i.e. how materials and interfaces deform) is still unclear.

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3.6 System level simulation

Current state of the art and challenges

The new dynamics of product development demand rolling out effective and efficient system designs in a short time span and with reduced costs, with the pressure of increased competition from market players. This requires that the time conventionally needed for conceptualization and validation of new designs has to be significantly reduced without having to compromise on the quality. In order to determine the optimized variant, it is necessary to evaluate its thermal, thermo-mechanical, and static response under varying material properties. This also helps in ascertaining the sensitive material parameters which influence the critical response. Finite element-based simulation plays a crucial role here in predicting system behavior under varying parameters. This method proves to be useful in delivering credible results within a short time span, thereby accelerating the design stage.

Virtual Design of Experiments (Virtual DoE) is an automated simulation methodology wherein the design space is composed of a range of properties (for a particular material) which are available in the market. A suitable model is considered for which the range of the properties to be evaluated are defined as the design space using a central composite faced (CCF) plan. Numerical simulation results for the defined points in the design space are input to obtain the response surface of the considered model. The response surface, such as deformation, stress, strain and strain energy, helps in determining the effect of each parameter. The degree to which each parameter affects the response determines the critical material parameters of the system. From this information, a judicious decision can be made regarding the materials properties for the components in a timely and cost-effective manner.

In order to predict quantitatively the stress state of design elements for an electronic control module, for example, several conditions must be fulfilled. First, a detailed geometry of all design elements must be taken into account. The geometry is typically validated by cross sectioning, X-Ray inspection or etching of the molding compound. Next, all the material properties must be assessed. For this purpose, materials are characterized on-site and the appropriate material models are developed. Finally, the boundary and load conditions must be well defined. For accurate prediction of thermo-mechanical behavior under active power conditions, the power dissipation in all design elements is taken into account. Thus, the simulation workflow starts with electrical simulation. The result from this step is taken as an input for the thermal simulation, to obtain the temperature distribution within the electronic control module. Next, the validated temperature distribution is used as an input to thermo-mechanical simulation. Based on the predictions of the thermo-mechanical model, the stress/strain analysis of the ECU under real working conditions is performed. This sub-modeling technique allows a quantitative estimate of a stress state in a design element. That enables a risk assessment for different failure modes.

Potential Solutions

In recent years there has been an upward trend in the usage of microelectronic components in almost every industry sector. The usage of Electronic Control Units (ECU) and integrated circuit (IC) packaging plays a crucial role in accommodating this growing trend. With more advanced highly automated and autonomous features set to be incorporated in the future, developing smart electronic systems seems to be the way forward. To achieve a competitive edge, the solution undertaken to deliver these devices in the market must be cost and time effective. Finite Element (FE) based simulation is one such technique employed to achieve this goal. With the results of simulation, an insight into the behavior of the system is obtained, which helps in making judicious development decisions [1]. Conventionally, simulation is used during the verification and validation stages of product development, i.e. at the end of the design cycle. By making use of simulation in earlier stages, numerous design-analysis iterations can be performed in a timely manner, thereby zeroing in on the optimum variant economically [1]. Acceleration of the design process of each new electronic smart system or IC package can be achieved by utilizing a simulation-driven design concept, e.g. to define the bill of materials before the first prototype is manufactured. The numerical models from simulation serve as a good beginning for divergent activities such as sensitivity analysis and generation of concept candidates [2]. Specifically, Virtual Design of Experiments (VDoE) is a potential technique that allows pre-selection of materials for the designed system. This ultimately allows for system optimization based on the tool chain tolerances and deviation in material properties (e.g. variation of modulus of elasticity or coefficient of thermal expansion).

Virtual DoE: It has been shown that by augmenting simulation techniques with statistical and stochastic methodologies, manufacturers are gaining in terms of reduced time-to-market [1] [6]. The conjoint application of simulation and design of experiments with economic analysis aids in the decision-making process at a semiconductor company, which results in increased production [4]. This combination of methods emphasizes using simulation as a means to execute the designed experiments to determine the correlation between input variables and output responses. Virtual DoE [5] techniques allow optimizing the product's performance by varying the input factors which are responsible for its behavior. This stage helps in selection of optimum material type/geometric configuration for the chosen module [3] [6] [7] [8] [9]. This concept is demonstrated in an example: The Virtual DoE technique can be used to select a molding compound for an IC package. The important properties of a particular molding compound which influence the stress state in the IC components can be estimated. These properties are defined as factors/predictors in the experimental design. The range for each property is defined based on its characteristics available in the market. Based on the chosen design plan, test cases/data points are generated. The results of the simulation, giving the mechanical response of the electronic control module (or smart system), is used as input for regression analysis. Utilizing a quadratic model which considers the main parameter affect, as well as the cross-interaction affect, the response surface is generated.

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3.7 Reliability and Prognostics

Current state of the art & challenges

The history of reliability as we know it now goes back to the 1950s, when electronics played a major role for the first time [1, 2]. When creating new (integrated) functionalities and/or increasing the performance, the concerns of reliability and functional safety should be accounted for right from the start of development. This avoids wrong choices, which otherwise may lead to costly and time-consuming repetitions of several development steps or even major parts of the development. In the worst case, unreliable products could enter the market with dramatic consequences for customers and supplier. The main challenges in the electronics industry are related to [3, 4]:

- Continuous growth in number, complexity, and diversity of the functional features, of the devices and components integrated, and of the technologies and the materials involved in each product;
- Increase in reliability and safety level to be achieved by the products, which will simultaneously and more frequently be deployed to ever harsher environments;
- Decrease in time-to-market and cost per product due to the stronger global competition;
- Higher complexity and depth of the supply chain, raising the risk of hidden quality issues.

With the increasing amount of complexity, it is imperative for the reliability of heterogeneous integrated systems to move from standardized test-to-pass towards prognostics-based performance measurements, see figure 12.

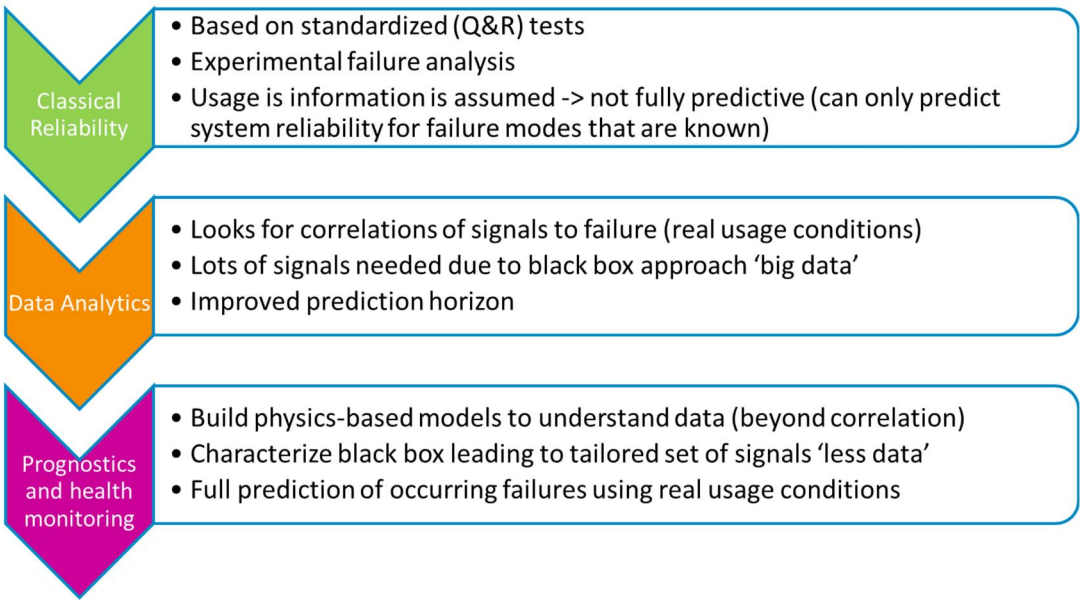

Figure 12: From standardized test-to-pass testing towards prognostics-based performance measurements.

In this migration, three significant improvements in reliability methodologies, as well as their prompt implementation and transfer into industrial practice, need urgent attention by the academic world, to keep up with heterogeneous integration product developments.

Predefined qualification plans are applied based on inherited standards, often without adaption to the specific new PoF situation, see also figure 9 [5, 6, 7]. We need to move towards deep understanding of possible failure modes, their associated mechanisms, and the inherent testing-to-failure to find them. Instead of testing to comply, engineers need to look for the weakest link.

While virtual schemes based on numerical simulation are widely used for functional design, they lack a systematic approach when used for reliability assessments. Besides this, lifetime predictions are still based on old standards (MIL, FIDES, Telcordia, etc.) assuming a constant failure rate behavior [8, 9]. Here, the so-called digital twin can prove useful; it is no more than a mathematical model of a physical object [10].

Prognostics and monitoring are not just about creating a more reliable product: they are about creating a more predictable product based on real-world usage conditions [11]. Data analytics is a necessary part of this, but is not enough [12]. To add value, product insights need to be leveraged into the technologies that are used to differentiate a product from others. Prognostics and monitoring are not about troubleshooting reliability issues; rather, they are a new control point enabled by the transition to a services business. It is the combination of data and deep physical (and technological) insight that will give a unique "right to win" in the industry [13]. The future possibilities for using big connected data in reliability applications are unbounded. Lifetime models that are based on this data have

the potential to explain much more variability in field data than has been possible before. Today, rarely any solutions at the component or system level are available except from high-end products (e.g., in avionics and energy infrastructure). Search for early warning failure indicators is still at a basic research stage. The ability to exploit data analytics on the huge data sets held by companies (based on past qualification tests) will also provide knowledge generation to support reliability [15].

Potential Solutions

Virtual prototyping is not new, but the application for reliability purposes needs urgent attention. Here the digital twin or virtual model of any product or device can be fed with testing results. The digital twin by itself should accurately describe the (failure) behavior of the product/device. The development areas that need to be addressed are listed as:

- Virtual testing – design of very harsh tests for component (and system) characterization (to find the margin beyond the qualification level, i.e., to determine the robustness)
- Mathematical reliability models that account for interdependencies (e. g., found by simulation) between the hierarchy levels: device – component – system
- Mathematical modeling of competing and/or super-imposed failure modes
- Failure prevention and avoidance strategies based on a hierarchical reliability approach
- Virtual prototyping – DfX – building blocks (covering one effect after the other)
- Simulation methodologies and approaches (including multi-scale, multi-field, chip/package- & chip/board-interactions, fracture and damage mechanics, reduced order and meta-models)
- Model library (digital twin) of the device for DfX (detailed models for manufacturability, reliability, and meta-models)
- Parameter studies (automatic DoE assessments, material modeling, case studies)
- DfX optimization schemes and tools based on AI and machine learning algorithms
- Standardization of simulation-driven DfX (enabling the transfer of simulation results but also of models, substructures, metamodels etc. across the entire supply chain)
- Automation of reliability assessment (component/module/system level end-of-life time predictions) based on electronic design input (i.e., prior to the 1st sample fabrication)

Prognostics and health management (PHM) is the next step from condition monitoring; it is not new by itself but needs to be fueled with ways to better manage large amounts of incoming data (known as data analytics). Generating data is easy – the key is to generate useful data. Development areas that need to be addressed are listed as:

- Self-diagnostic tools and robust control algorithms, validated by physical fault-injection techniques (e.g., by using end-of-life components)
- Hierarchical and scalable health management architectures, integrating diagnostic and prognostic capabilities from components to the complete device (incl. ‘smart redundancy’) and alarm management algorithms
- Monitoring test structures and/or monitor procedures (also: using available data) at the component and module level for monitoring temperatures, operating modes, parameter drifts, interconnect degradation etc. – according to the failure Pareto plot
- Identification of early warning failure indicators and development of methods for predicting the remaining useful life of the device in its use conditions (data collection, statistical assessment, prediction models)
- Merging of PoF based and data driven PHM approaches [14]
- Development of schemes and tools using machine learning technique and AI for PHM
- Big sensor data management (data fusion, finding correlations, secure communication)

Currently, PHM has been implemented to solve many engineering problems (e.g., failure diagnostics, lifetime estimation, and reliability prediction) with multi-disciplinary approaches that include physics, mathematics, and engineering. However, most current PHMs are primarily implemented in physical space, with little connection to a virtual model. A digital twin (DT), see figure 13, can provide a virtual space (digital mirror) of the system to depict the behavior of the real entity. Normally, the DT is modeled in three dimensions, i.e. the physical entity, virtual model, and connection [12]. A DT-driven PHM includes a five-dimensional architecture with physical model, vertical model, data model, service model and connection model. It makes effective use of the interaction mechanism and fused data of the DT. The development areas that need to be addressed are:

- Predictive reliability modeling and simulation-based optimization
- Multiphysics/multiscale/probabilistic dynamic simulation

- Full lifecycle in-situ monitoring with smart sensors
- Big-data storage with Cloud and processing with deep learning
- Intelligent decision-making with AI
- Intelligent perception and connection technology
- Digital twin data construction and management
- Smart service analysis method based on digital twin data
- Testing strategy and testing platform for verification, i.e. cost-effective testing strategy and test methodologies; automated test pattern generation, data analysis and diagnosis flows; multifunctional performance testing; multi-scale testing; multi domain cross talk; complex system testing
- Smart software
- Cyclic economy management

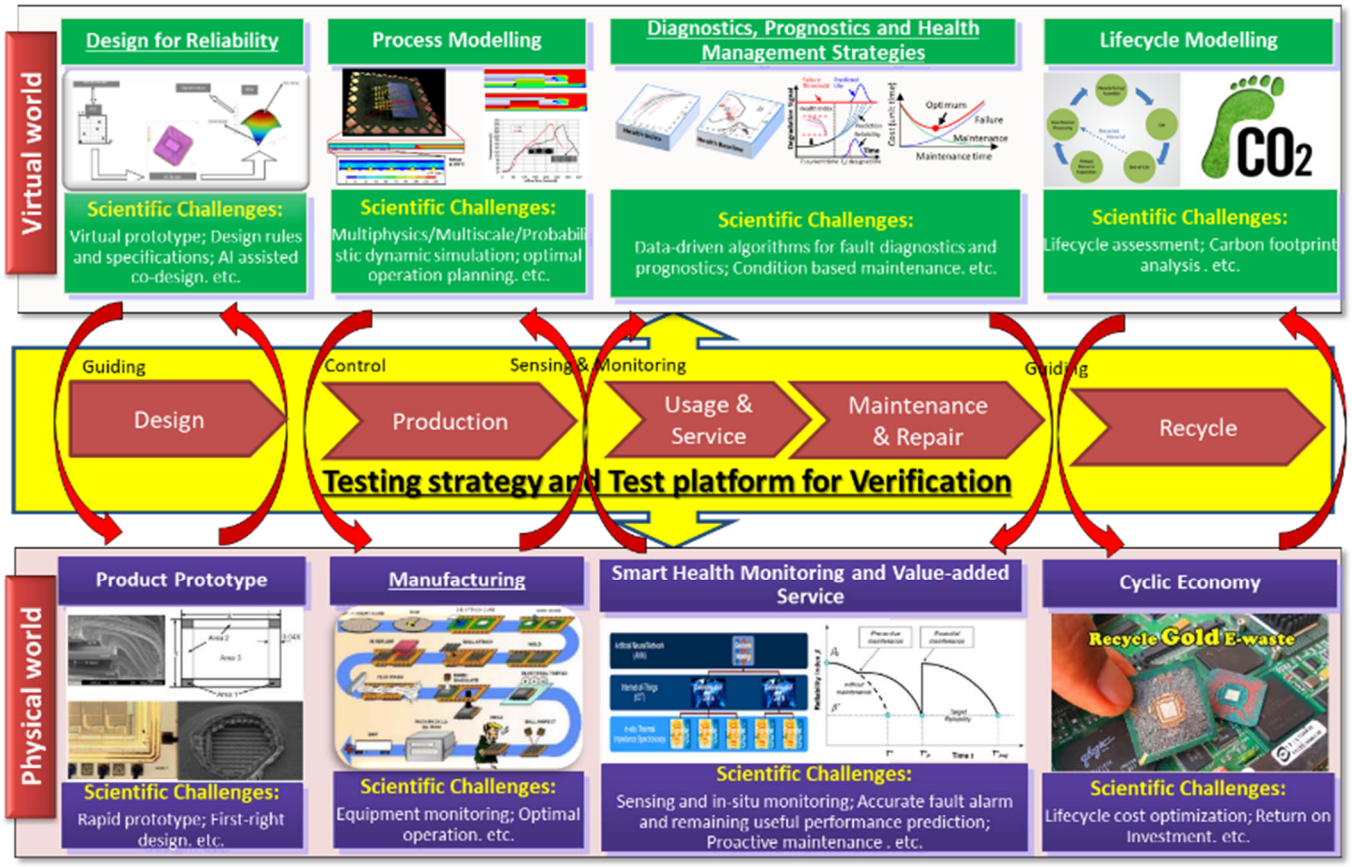

Figure 13: Digital twin for electronic components and modules (Source: G.Q. Zhang & Jiajie Fan)

All development areas listed above can only become available if they are put on a time scale. In this section, the areas are projected towards a time scale in years, being 3 – 5 – 10 years. This horizon is listed in table 2 below.

Table 1. Modeling & Simulation Metrics

Metric	5 years	10 years	15 years
Concept to Product	5 years	3 years	18 months
Model Accuracy for Reliability	50%	75%	100%
Products validated through M&S	50%	70%	100%
AI/Machine Learning	Use of Machine Learning to learn from different designs for single physics	Use of Machine Learning to learn from different designs for multi-physics	
Multi-Physics	Accurate multi-physics analysis for chip-package co-design		Accurate multi-physics analysis for whole system

Data Sharing	Interfaces between tools and ADK's and PDK's	Data and model sharing through supply chain

Table 2: Key developments and achievements required for PoF, DfR and PHM

Achievements			
Year	**PoF**	**DfR**	**PHM**
3	• Physical failure analysis techniques applicable during the loading situation • Realistic material and interface characterization depending on actual dimensions • Variability and uncertainty: multi-objective optimization, stochastic methods, I4.0	• Chip / board / module / system interaction: standard definition for tool chain and data exchange format across supply chain • Virtual testing – design of very harsh tests for component characterization • Metamodeling and Model Order Reduction: complex behavior of a system incl. stochastic data	• Self-diagnostic tools and robust control algorithms • Artificial intelligence and machine learning: usability in daily engineering tasks • Prognostics using hybrid approach (combined data and model driven approach)
5	• Comprehensive understanding of top-25 failure mechanisms incl. prediction models • Digital twin: Understanding of field related failure modes • PoF models considering aging	• Mathematical modelling of competing and/or super-imposed failure modes • Failure prevention and avoidance strategies • Virtual prototyping – DfX – building blocks • Metamodeling and Model Order Reduction: non-linear behavior using machine learning • Automation of reliability assessment	• Hierarchical and scalable health management architectures, integrating diagnostic and prognostic capabilities from the components to the complete device • Monitoring test structures and/or monitor procedures • Development of schemes and tools using machine learning technique and AI for PHM
10	• Accelerated testing methods based on mission profiles and failure data • Multi-mode loading based on mission profile • Digital twin: Local/global key failure indicators	• Metamodeling and Model Order Reduction: Multi-objective optimization (design, manufacturing, costs) • Model library (digital twin) of the device for DfX • DfX optimization schemes and tools based on AI & machine learning algorithms	• Identification of early warning failure indicators and development of methods for predicting the remaining useful life of the device • Digital twin: In-situ state of health evaluation • Big sensor data management (data fusion, find correlations, secure communication)

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