2021 Edition

Chapter 14: Modeling and Simulation

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1. Executive Summary

The 2021 edition of the HIR modeling and simulation chapter contains several updates to all sections detailed in the 2020 edition, as well as new sections. 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 details how these tools will support the knowledge base for these systems, as detailed in Figure 1.

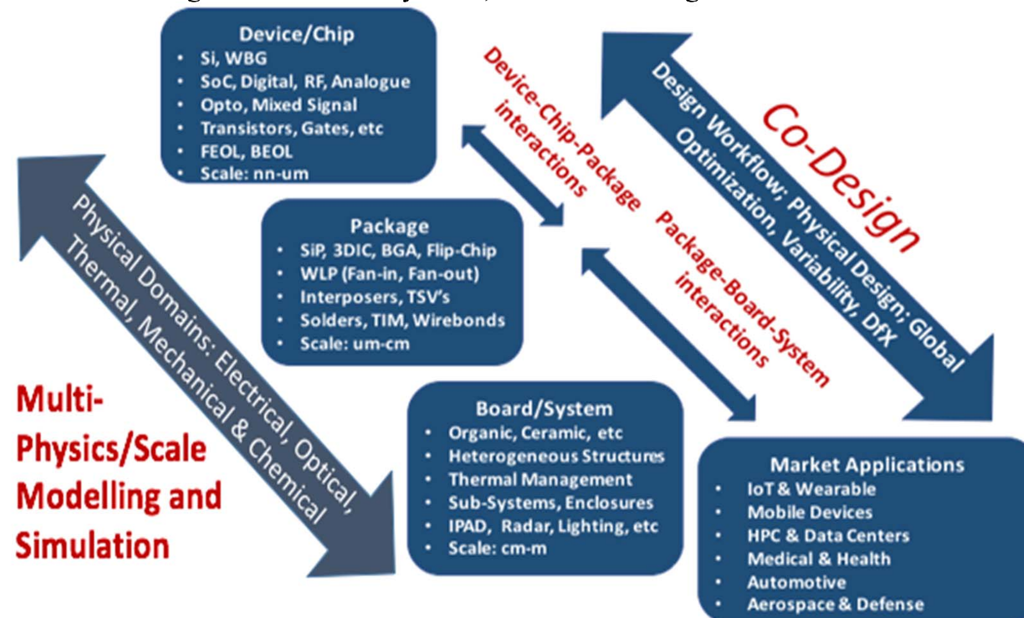

Figure 1: Supporting the Knowledge Base for Heterogeneous Integration

Analysis using M&S tools today can generally be classified as being single physics (electrical, optical, thermal, mechanical, chemical) and 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 are 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 generally, the die electro-thermal behavior ignores complex board behavior and its constraints). For integrated heterogeneous systems, such assumptions will become invalid.

2. Scope

The Modeling and Simulation TWG considers challenges and potential solutions that are detailed in this chapter under the following headings:

- ***Modeling and Simulation Techniques***: State-of-the-art, challenges, and potential solutions
- ***Applications***: State-of-the-art, challenges, and potential solutions

Under the heading ***Modeling and Simulation*** **Techniques**, section 3 covers the challenges for designers and the actual modeling and simulation methodologies. This is focused on (1) Electrical, (2) Thermal and Themo-Mechanical, (3) Molecular Modeling, (4) Mechanical and Multi-Physics, (5) Multi-Scale, (6) AI and Machine Learning, (7) System-Level Analysis, and (8) Materials Characterization.

Under the heading ***Applications***, section 4 provides details of the challenges and potential solutions for modeling and simulation for applications and aims to align with other chapters in this roadmap where modeling and simulation can support the challenges detailed in those chapters. For the 2021 edition of this chapter, these application domains

are (1) MEMS and Sensors. (2) Manufacturing process models, (3) Composite Materials. (4) Reliability, and (5) Digital Twins.

In addition to the taxonomy of the modeling and simulation categories listed above, the chapter also focuses on articulating the key metrics (see section 5) 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 modeling and simulation capabilities will become critical for supporting product development and design flows (See Figure 2) across the chip-package-board-system domains. These design flow challenges will be captured for each of the domains and related to the key device-, packaging-, and system-level challenges, in particular in Chapter 13 on Co-Design.

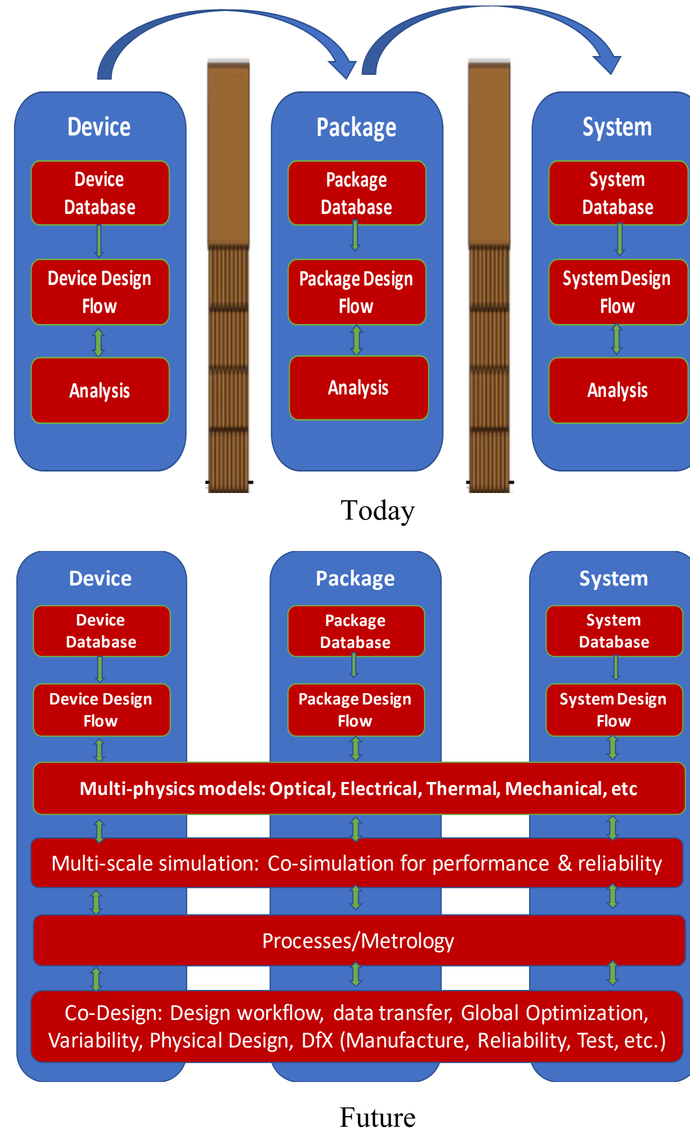

Figure 2: Moving towards a new M&S paradigm

3. Modeling and Simulation Techniques

Different levels of abstraction can define modeling and simulation tools, from circuit simulators such as SPICE to computationally complex models using molecular dynamics, finite elements, and computational fluid dynamics. Traditionally, systems designers undertook the thermal and mechanical analysis, passing on the requirements/constraints to package designers. Chip designers mainly focused on electrical analysis, which is very challenging for highly detailed system-on-chip designs. But chip design can no longer avoid thermal and mechanical stress issues, 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. Modeling and simulation must address the need for modeling chip-interactions at the nm scale (e.g., transistors), package interactions at µm-mm scale (e.g., TSV, micro bumps),

and mm-m scale for systems (heat sinks, PCB's, 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 are 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.

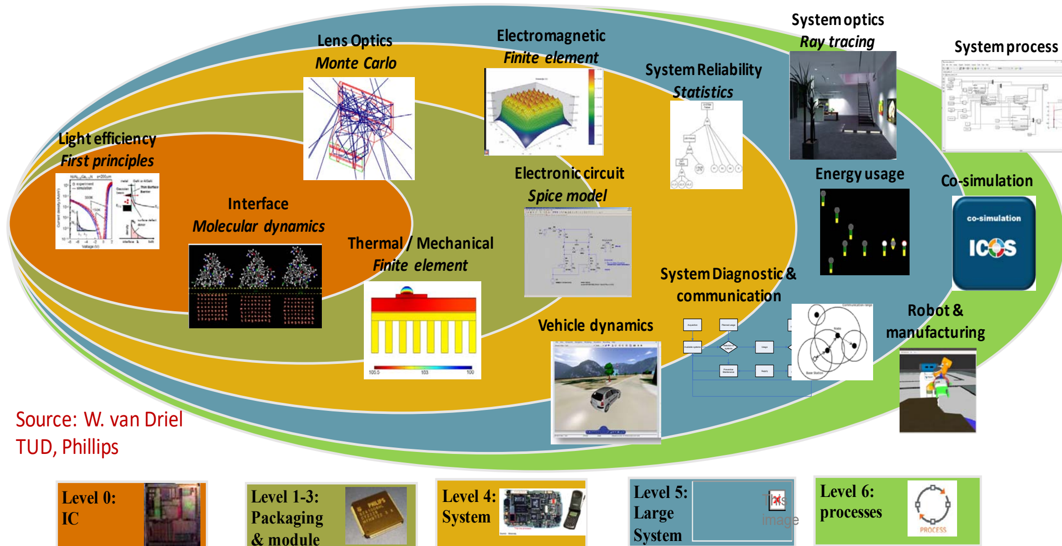

Figure 3: Modeling and simulation landscape for photonics

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 illustrates the overall vision for modeling and simulation and how it will inform the knowledge base for advanced packaging and heterogeneous integration.

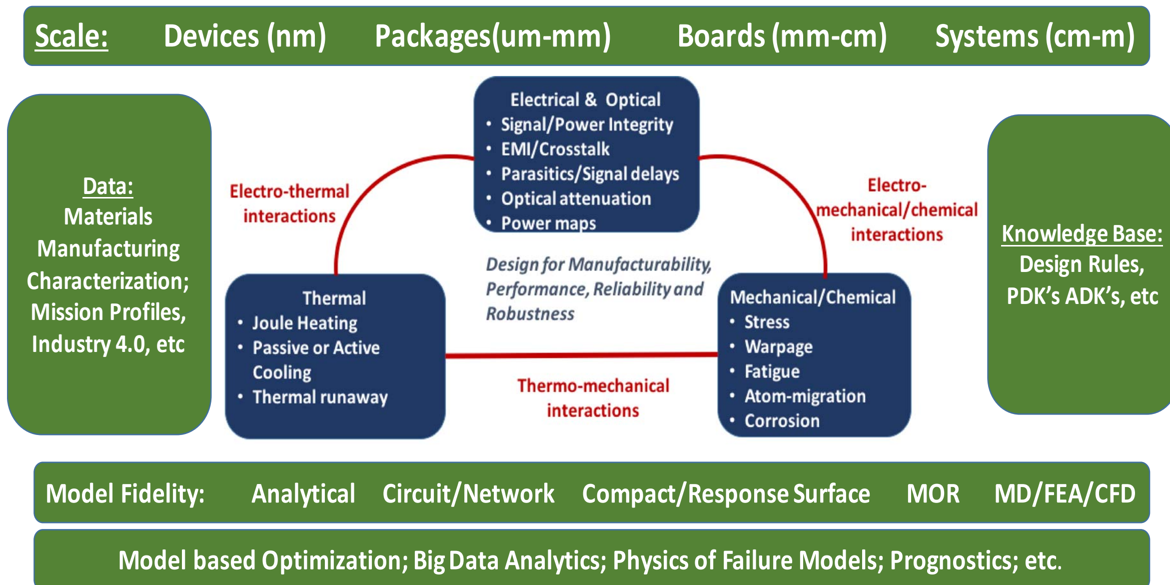

Figure 4: Modeling and simulation to inform the knowledge-base for heterogeneous integration

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 in modeling and simulation techniques and identify key challenges to overcome.

3.1 Electrical Analysis

Current State of the Art and Requirements/Challenges

To fully understand the electrical design challenges of electronic systems with heterogeneous integration, one needs to evaluate the current methodology, analysis capability, and limitations for non-heterogeneous (i.e., individually-packaged) components. The electrical analysis focus for the electronics IC packaging engineer is timing, signal integrity, power integrity, and electromagnetic (emission and immunity for both radiated and conducted). In addition, the multi-physics consideration, depending on the complexity, may include electrical, thermal, and mechanical interactions for digital, analog, and mixed-mode designs.

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 (i.e., their figures of merit) of concern. For example, a silicon die includes billions of interconnect segments on a micrometer-level scale, with dimensions much 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 with Joule heating of milliwatts per square centimeter.

Currently, the details of the electrical analysis are customized for each component. The signaling interconnects analysis is dominated by RC delay, resistive loss, crosstalk, and signal delay at the semiconductor level. However, the loss due to the dielectric loss tangent and copper roughness at the printed circuit board level becomes significant. A sub-micron scale is needed for extraction at the semiconductor level, while the scale is much larger for the printed circuit board. However, sub-nanometer-level roughness is required for surface impedance formulations in a printed circuit board. The methodology for extracting these details is facilitated by an independent analysis of each component level and creating specifications and budgets to communicate with the adjacent levels. Therefore, the electrical analysis can be performed one component level at a time.

For the semiconductor die, where the physical structures are smaller than a wavelength; quasi-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 quasi-static simulators support SPICE equivalent circuit models' generation, which can then be used in chip-package circuit-level SPICE simulators.

For printed circuit boards, where the structures are larger than the wavelength, high-frequency analysis that includes the electric field and magnetic field coupling is required. Such analysis requires using full-wave 3D field solvers to solve the wave equation from Maxwell's Equations directly. High-frequency behavior such as transmission line effects, attenuation and dispersion due to losses, skin and proximity effects, 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. However, for high-speed channels with serial components, 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 designed on very different schedules by different teams for non-heterogeneous designs. For example, 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. The packaged semiconductor design is likely completed before the printed circuit board design. The silicon design team would have been redeployed before the printed circuit board design began. Even if co-design could be done, it would not improve the semiconductor design or optimize the design across the package hierarchy since the semiconductor component was already

manufactured. A broadly segmented supply chain has to be developed to support this design model. Additionally, the current component-level centric design methodology is compartmentalized (i.e., each component is designed separately with little to no communication between each team). This "throw-over the wall" hierarchical approach is liable to failure.

The state-of-the-art heterogeneous integration electrical analysis currently depends 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 heterogeneous 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 early in the design phase. 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 essential for analyzing the critical performance parameters of the completed design. It is also helpful for verification, validation, 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 if 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 genuinely open standard should be a long-term industry objective. Sharing geometrical descriptions of components that the designer considers proprietary is limited 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. A simple example is analyzing the impact of temperature excursion on one component, impacting the metal resistance in another component without divulging the proprietary design details.
- The standardization of the compliance specification can start with current standards for robust channels such as PCIe or SAS. Future standardization can include the previous two points of interface files and physical geometrical information. Still, 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, voltage and temperature circuits, 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 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, the noise and jitter impact is budgeted and sensitive components are isolated from noisy components to ensure proper operation. 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 is needed to confirm isolation than what may be required. In addition, when functional issues are discovered with hardware operation, simulation is of limited use in diagnosing unexpected electrical behavior.

Potential Solutions

Future co-design and co-simulation need to address multiple physical components, as discussed above. Compared to a printed circuit board, the scale of features both in size and number in a semiconductor device highlights the challenge. 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. For robust design, behavioral models of switching circuits, signal and power distribution networks, and noise susceptibility are needed. As the integration capability advances with embedded devices, stacking and TSV interconnection of devices, and increasingly sophisticated interposer and redistribution wiring technology between devices, the design, simulation tools, and methodology need to stay in step. Specifications will be developed during the five-year horizon, and efforts will be made to define further the tools and methods for analysis for companies working cooperatively to specific standards. In the five- to ten-year period, the methodology could develop into sharing designs more broadly through 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 and electrical analysis tools will reflect how the industry has developed. These tools will need to integrate the components as this part of the industry seamlessly has matured, and differentiation may come from cost and the ability to integrate the capability to meet the desired needs. Integration of electrical and thermal analysis will progress during the near term. Electrical-thermal co-simulation needs to handle increasingly detailed simulation on a single package or component level. 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 electrical and thermal response interaction 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 coupled multiphysics and system co-design methodology across devices where details can be specified and shared, say in a consortium. In the longer term, the methodology needs to accept proprietary devices and not be restrained to closed design communities to exploit the potential capability of heterogeneous integration.

Power and signal integrity traditionally have different physical boundaries 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. For a package design, a power integrity simulation may be of most interest in the tens of megahertz to gigahertz range. The noise in the power distribution created by switching circuits of adjacent components needs to be included in the analysis, increasing 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.

Power integrity analysis needs to be increasingly integrated into signal integrity analysis. The combined signal/power integrity electromagnetic interactions are critical for designing high-speed and high-performance IC packages and systems. Impact of power distribution network (PDN) design to high-speed parallel/serial interfaces (viz SSN, coupling to signal trace, among others) and natural anti-resonance cavity of PDN impact to emission and immunity are all combined effects that need to be considered [4-5]. Additionally, the development and standardization of compact models will be essential to capture the coupled power and integrity electromagnetic interactions accurately. 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, emission, and immunity;
- 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.

Power delivery is of utmost concern when optimizing dielet interconnection within a package. Therefore, integrating modeling and simulation capabilities in the co-design tools to handle the physical placement of dielet power and signal bumps, along with integrating decoupling capacitors, is highly desirable. Additionally, the modeling and simulation tools ought to optimize power per bit needed to meet data rate objectives for optimal system-

level performance. Furthermore, the simulation capability of dielet wiring that takes the system performance constraints and can 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.

The development of modeling and analysis methodologies creates the opportunity to apply machine learning, deep data analysis, and multiscale domain decomposition methods to solving concurrent multiphysics and system co-design (Figure 5). The coupled multiphysics and system co-design (MSC-D) approach will provide for modeling and analyzing the interactions between the die, package, and PCB system, while concurrently addressing the multiphysics interactions.

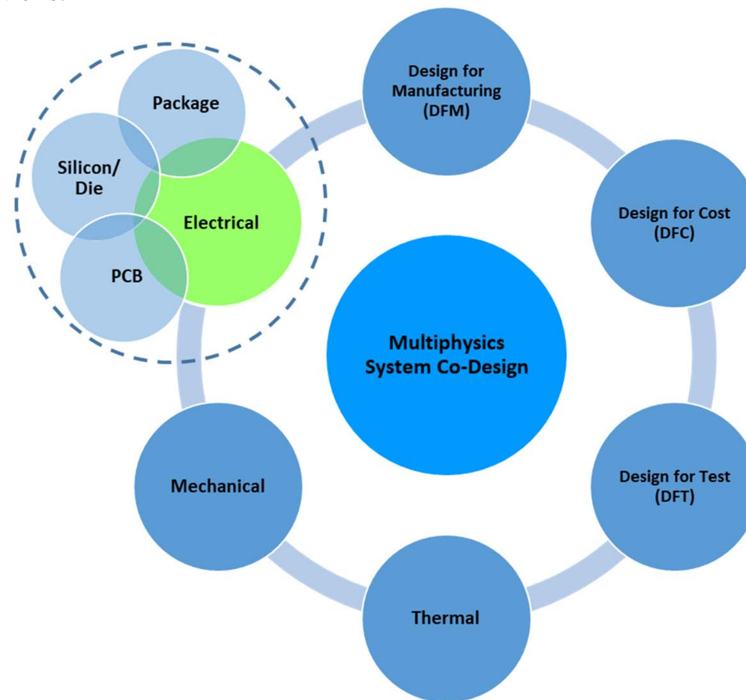

Figure 5: Coupled Multiphysics and System Co-Design (MSC-D) Modeling and Analysis Methodology

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. Then, for the middle term of five to ten years, expand the techniques to the approximate response of co-analysis techniques. Independently, the ability to analyze across multiple components will likely be feasible. In the long term, combining the ability to explore the design space for co-analysis and multiple components is a goal.

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

The functionality and performance of heterogeneous problems are increasingly dependent on the coupling of various physical phenomena on different scales in both time and space. Solving these problems numerically is computationally exhaustive if accurate solutions are desired from the complexity of the multiple physical phenomena. Complexity is exacerbated with the need for multiple iterations to achieve optimal performance. Recent development and progress in parallel domain decomposition methods (DDM) have substantially improved the capability of numerical computational techniques (viz. FEM, MoM, FDTD) in solving multi-domains and multiphysics large-scale problems [6-7]. DDM divides a large problem into multiple smaller yet manageable subdomains and conquers each individually. The decomposition renders the original problem less complex and more efficient in terms of memory usage and parallelization. Current ongoing research and development work focuses on addressing the multiscale need for heterogeneous coupled multiphysics and system co-design. Solutions are achievable by combining DDM with other decomposition algorithms (e.g., proper generalized decomposition) methods. These developments are

laying the foundation to address the computational challenges encountered in the proliferation of realistic heterogeneous systems.

System performance metrics create 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 more systematically, 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 the verification of the design before tape-out, and aid in characterization and diagnostics during system run time.

Ultimately, with the emergence and adoption of concurrent system co-design coupled with multiphysics considerations, a unified approach to design and optimize heterogeneous integrated systems is reachable with ongoing research and technological progress to close current and future gaps (See Table 4 in Section 5). Advances in standard file sharing format, interoperability between tools, multiscale algorithms, and global specifications and standards will successfully enable the adoption and proliferation of the unified MSC-D modeling and analysis methodology.

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3.2 Thermal and 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 are 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.

The thermo-mechanical interaction between chip and package (CPI) and also between package and board are considered to be crucial to guarantee a ILD fracture-free package assembly and in operation. Attempts for CPI modeling have been done by several key players but remain challenging due to the large-scale difference (from nanometer to centimeter) [8,9]. For more performant modeling, advances are needed in the use of compact models and automated local-global simulation, allowing for covering the different dimension scales. Accurate material properties as input for the models are still marginally available. Dedicated measurements of stiffness, CTE, and strength of low-k materials are needed. A positive development is that more and more stress sensors are integrated at the chip level, which allows for validating the simulation models – for example, the stress after flip chip assembly [10]. This allows following the stress build-up during the package assembly. In operation, it can be used to monitor the IC for possible local fractures as input for the PHM of the system. Also, strain measurements using DIC methods are a suitable approach to validate the models, even measuring local effects.

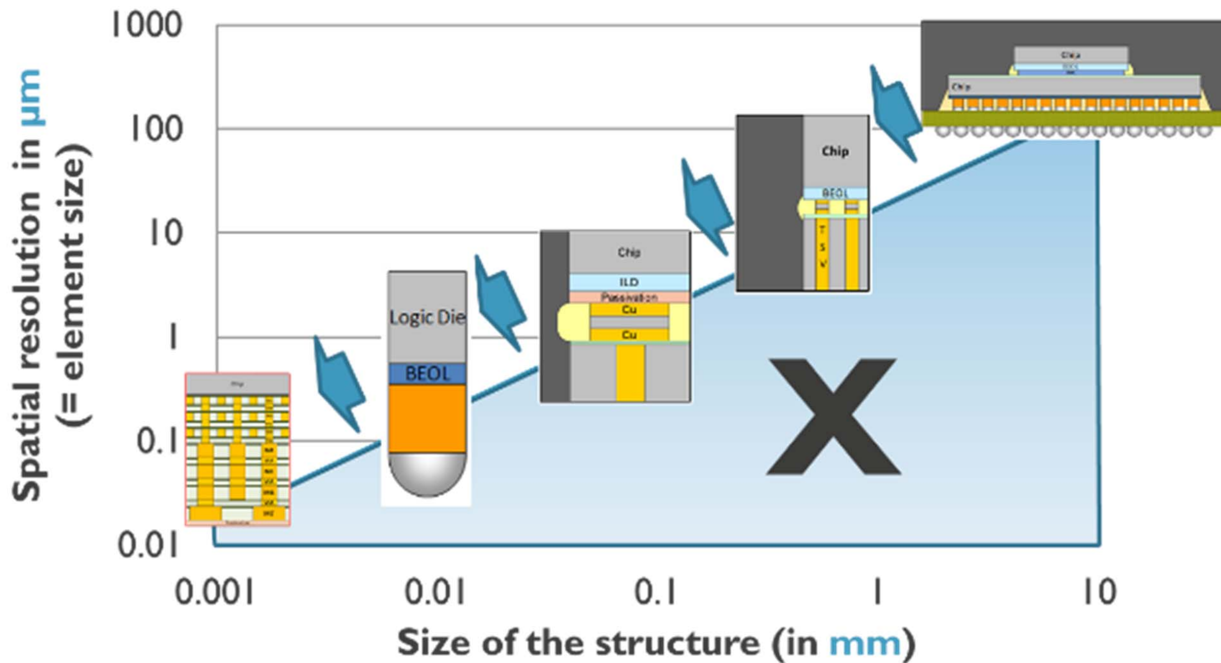

Figure 6: CPI: from nano to cm level simulation challenge

Potential Solutions

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 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 feed-forward 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.
- Automation of local-global simulation for CPI studies using compact models. Starting from the local level with all details, compact models are generated to be used in the higher level models. And this should

work in the two directions, so large-scale results need to be transferrable to what happens at a nano-scale level.

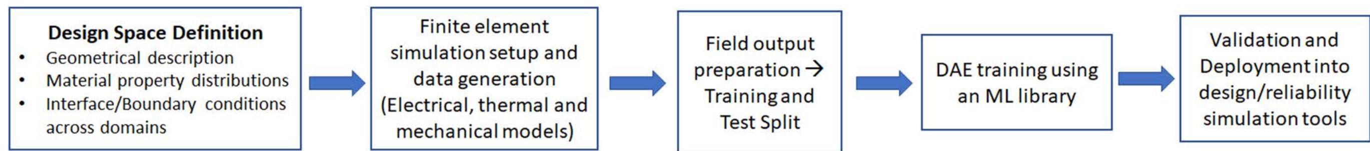

Figure 7: Integrated FEAA and Machine Learning for Thermal Management

One example of such deployment in the thermal domain is by Zhang et al [4] (see Figure 7) who apply machine learning to real-time thermal prediction/management and demonstrate improved accuracy, as well as significant runtime overhead reduction.

Importance of Accurate Material 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 a 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 materials models (with the specification of uncertainty) into multiphysics modeling tools to generate a comprehensive training set which is then put into machine learning frameworks to enable rapid design space definition, such as that shown in the workflow above (see Figure 7).

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3.3 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, 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 (or the "molecular-mesoscale" level, calculating higher-size-order interactions from parameterized molecular groups or particle beads). The energy relationships for both bond and non-bond interactions in the atomic force-field methods have been pre-parameterized using either direct spectroscopic measurements or from quantum calculations. The parameterizations for molecular-mesoscale models can be determined either from measured properties (like solubility), or calculated from the quantum or molecular dynamic level.

The molecular-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 8, showing different levels of coupling into the cohesive side of an adhesive interface at failure, depending upon the type of deformation. There is a limitation of scaling to the molecular-mesoscale method as most commercial packages use particle bead parameters that represent the size of a functional group (~5A bead particles). However, studies (Figure 8) [2,3] have found that a bigger particle can be used if the geometry of the bead interaction is considered and interactions are consistent with the shape of the bead. For instance, the particle beads for the polymer shown in Figure 8 represent an entire repeat unit size (~25A diameter), using a spherical particle bead and parameterization focused on the energies of the repeat unit bead. Conceptually, the particle beads can be extended to different shapes depending upon the geometry of the molecular group that will be used as the basis of the particle.

One way to help extend molecular modeling beyond the "molecular-mesoscale" is by use of molecular models to determine generalized interaction energies of the larger macro-scale particles. For example, higher scale (length and time) Discrete Element Models (DEM) have been used to explicitly represent silica filler particles and their flow during underfilling using proprietary silica particle size distribution (PSD) blends in an underfill where the binder influence included in the model was determined by silica-binder interaction energies derived from molecular models [3,6]. DEM simulations have also been used to determine optimum PSD for best packing of silver flake in die attach [3,7].

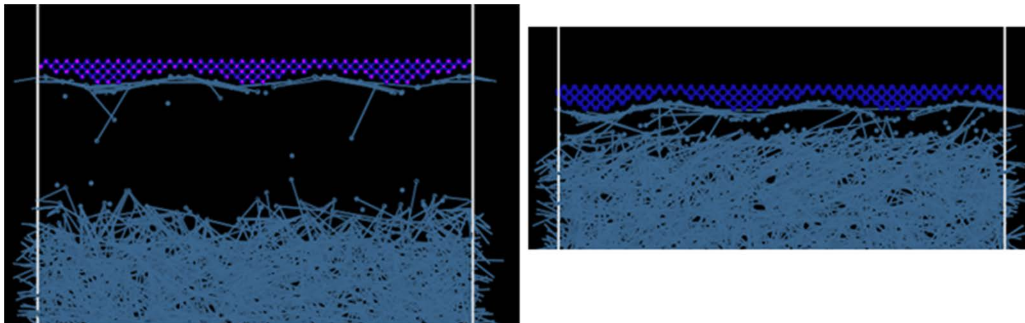

Figure 8. 3D Molecular-mesoscale interfacial failure for a roughened (sawtooth) copper oxide-epoxy adhesive interface, for pure tensile deformation (left) and pure shear deformation (right)2,3 showing higher coupling into the cohesive side for the shear case (sides shown are ~14nm wide).

Today, quantum-level programs, on a practical level for industry needs, employ density functional theory (DFT), which 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, interest 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 readily employed today for most organic and silicone systems as parameterizations (forcefields) are available. 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 sold 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. As with all quantum level calculations because of the nanoscale features and picosecond timescales represented, scaling the calculated to the observable is still an issue, but molecular models can still be used to parameterize and inform the larger molecular or mesoscale models which can be entryways into macroscale parameterization, as suggested in the underfill study.

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 fields 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 and can be very useful in understanding cure and aging. 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. Molecular modeling can potentially influence higher-scale models by defining when property transitions could occur depending upon condition (temperature, pressure and time or chemical rates). 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, available workflows 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). Both time and length scaling will be especially important to quantitatively extrapolate the molecular (and atomic) scale to the bigger realistic scales.

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, although how the neural net will treat issues of time domains (i.e. how materials and interfaces deform) is still unclear.

Another emerging computational area is that of the quantum computer. For molecular modeling, the use of quantum computing is still in its infancy as new codes must be developed around the new architecture and which also deal with issues surrounding the complexities of quantum computer errors. However, because of enhanced speed it is envisioned as one of the tools of the future that can help bridge the quantum to macro-scale gap as well as offer increased speed for other computational areas.

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3.4 Mechanical and Multi-Physics

The 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 (stresses contribute to the 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 (TSVs).

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 that 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 9. 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].

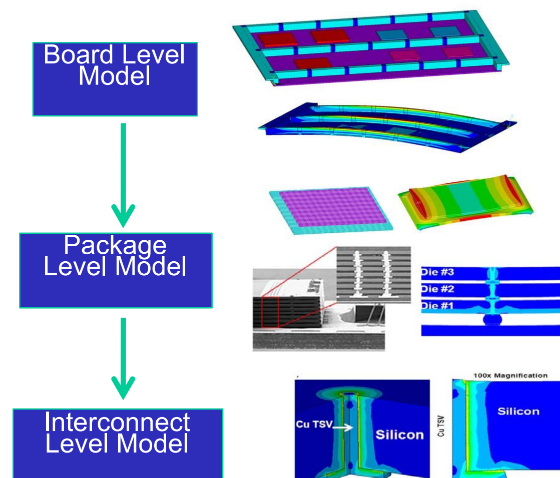

Figure 9: Mechanical (Vibration) chip-package-board design

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, hot spots and uneven temperatures will arise in the system due to Joule heating. 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 mechanical simulation focuses on the thermal stress due to thermal mismatch only (an 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 is one of the critical reliability issues in electronic devices, which is an enhanced mass transport process in the current-carrying metal induced by the driving force (electron wind) generated by the 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 conditions (see Figure 10 (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 the 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 Figure 10(b)). These forces result from different physical causes, such as the gradients of atom concentration, electron wind, temperature gradient, and mechanical stress gradient. For electromigration to be analyzed, self-diffusion, thermal migration, and mechanical stress migration must be coupled with electromigration for an accurate prediction.

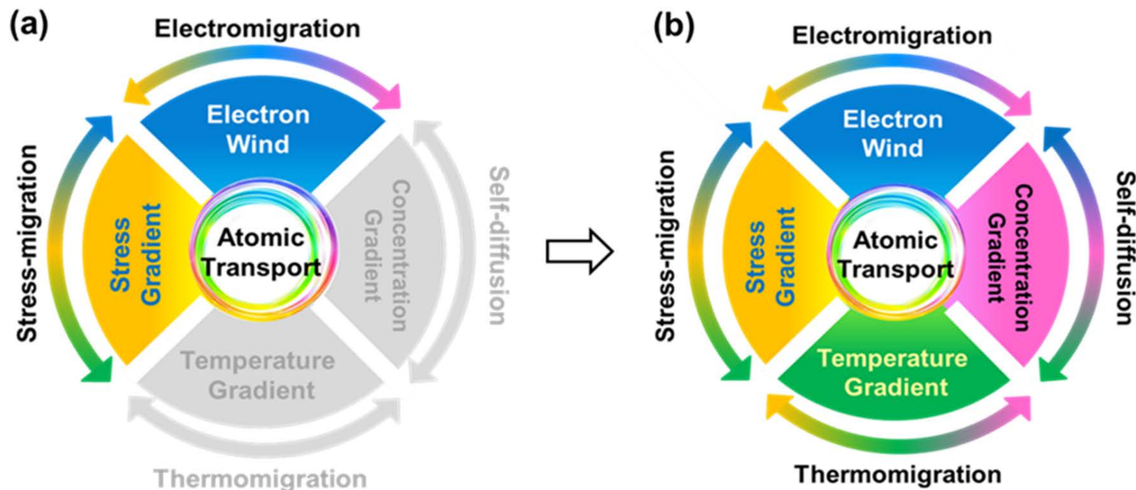

Figure 10. Interrelations among electromigration, thermos-migration, the self-diffusion, and stress-induced migration.[6]

In past decades, there have been many studies 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, such as micro-bumps/pillars, hybrid bonding, RDL and TSVs, 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 5.4×10^5 A/cm^2 to 6.0×10^6 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 solution to reduce the rate of electromigration at high temperatures is practically 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 11 shows the physics domain involved in the multi-physics modeling for a heterogeneous system.

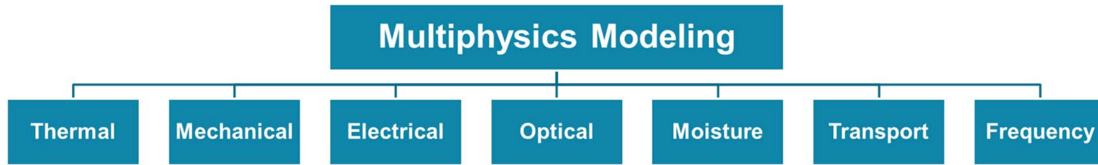

Figure 11. Multi-physics for a heterogeneous system

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 the 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 12 shows the evolution of the microstructure of a copper metal line for different technology nodes.

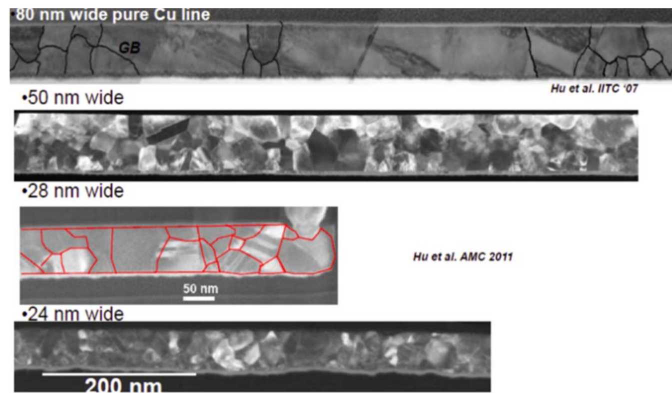

Figure 12. Copper metal line scaling over the past generations of CMOS technology

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. In summary, the main challenges in mechanics and multiphysics modeling are in the following areas:

- Continuous development in a heterogeneous system with more physics involved, such as in silicon photonics systems with optical modeling, in high power electronics systems with solid-fluid interactions, and in RF/radar/antenna systems with electromagnetic coupling.
- Complexity in new materials that exhibit highly nonlinear and non-conventional behavior and the feature size reductions that result in size-dependence and the challenge in determining materials properties.
- Uncertainty, higher complexity and variations in manufacturing process that lead to stochastic and complex behaviors in a system.

- Efficient and effective simulation tool development that tackles the modeling at multiple levels, from chip and package to board and system, combined with multi-scale modeling, as well as prognostics and health modeling.

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 is important. Further work is required to transfer data from metrology into modeling tools (see Figure 13), and there is a lack of consensus on accurate constitutive models used – for example, for non-linear materials such as solders.

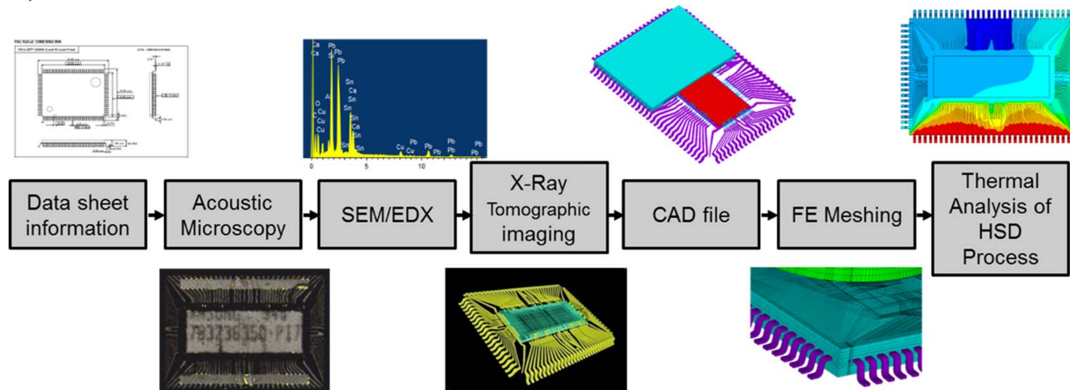

Figure 13. Integrating metrology with modeling

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 – 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 Modelling 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 layer 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, intermetallic properties 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 and deriving failure modes and criteria is another important area to achieve simulation accuracy, which is a basic prerequisite for tools like 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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3.5 Multi-Scale Analysis

There are many examples of multi-scale phenomena that are important in heterogeneous integration:

- Nanoscale phenomena at the device level. Examples include:
  - effects of strained-silicon mechanical fields and phonon interaction fields on channel mobility
  - leakage currents due to tunneling of 'hot' electrons
  - interfacial molecular bonding at metal-polymer interfaces
  - electron-phonon and phonon-phonon interactions in nanoscale heat transport in IC devices
  - enhanced nanoscale self-heating in FinFET and Gate-All-Around (GAA) technologies
- Microscale and mesoscale phenomena in package elements and interconnections. Examples include:
  - mobility and performance of GaN devices in the presence of threading dislocations
  - electromigration and thermo-migration in copper traces and in solder interconnects in the presence of grain boundaries
  - constraint cavitation in aluminum metallization in the presence of local stress gradients
  - thermo-mechanical performance of few-grained solder interconnects
  - dendritic growth and electro-chemical metal migration due to moisture and electrical bias
  - interdiffusion, intermetallic growth and Kirkendall voiding at temperature
  - effective PWB properties in the presence of localized fiber-matrix debonding
  - mechanical response of micro-porous sintered silver materials
  - grain-scale mechanical response of small metallic structures (copper or aluminum traces, solder joints, etc)
  - thermal contact resistance at thermal interface materials
  - electrical contact resistance between gold contacts in connector pins
  - thermal transport and electrical transport in filled conductive adhesives

- moisture transport in filled epoxy underfills and mold compounds
- Macroscale continuum-scale phenomena in electronic systems. Examples include:
  - Fourier thermal transport in heat sink structures
  - continuum scale thermo-mechanical chip-package interactions (CPI) and package warpage due to thermal expansion mismatches between die and other package elements
  - classical moisture transport by diffusion through bulk homogenized polymer materials
  - classical Maxwell fields in RF circuit elements

Current State of the Art

Modeling and simulation methods in heterogeneous integration have to span many orders of length and time scales, to successfully capture the important phenomena and design problems listed above from the nanoscale to the macroscale. Figure 14 shows a schematic of the computational approaches available today at the different hierarchical scales:

- Nanoscale level discrete methods [1, 2]:
  - 'Exact' Quantum mechanics (QM) level: ab-initio and first-principle solvers for Schrodinger's wave equation
  - 'Approximate' QM methods: Atomic orbital (AO) approaches and density functional theory (DFT) approaches
  - Discrete molecular level: classical molecular dynamics (MD), Monte Carlo (MC) approaches, coarse-grained molecular cluster modeling approaches
  - Particle level: Lattice dynamics (LD) approach in solids and Langevin dynamics (LD) approach in fluids
- Defect-scale level [3]:
  - Discrete dislocation dynamics (DDD) approaches
- Microscale level continuum methods [4-7]: Scale-dependent enriched-continuum mechanics (ECM) approaches for materials with microarchitecture (e.g. composite or porous heterogeneous materials):
  - Gradient-based methods
  - Nonlocal methods
  - Cosserat-type polymorphic methods
  - Doublet mechanics methods
- Mesoscale level continuum methods [8, 9]:
  - Grain-scale methods
  - Crystal-plasticity methods
- Macroscale level continuum methods [10,11]:
  - Statistical mechanics
  - classical continuum mechanics (CCM)

Computational approaches at all scales are based on variational approaches [12-14] and include finite element methods (FEM) [15], Galerkin methods, extended FEM (XFEM) and meshfree methods [16], and boundary element methods (BEM) [17]. Similar variational formulations for computational scale-dependent ECM approaches and discrete methods are also available in the research literature.

Hierarchical boot-strapped methods have been developed in the research literature, where higher length-scale models (such as XFEM for effective continuum models) have been developed, with input effective material properties estimated from lower-scale molecular or atomistic methods. As an example, mechanical and thermal system simulations may benefit from materials properties such as phonon dispersion curves obtained from LD approaches and defect energy potentials obtained from DDD models. The LD and DDD models, in turn, may rely on equilibrium configurations obtained from MD simulations, which in turn can rely on molecular potentials and force fields estimated for atomistic AO methods or DFT QM methods. Hybrid quasi-continuum methods are also popular in the research literature, relying on continuum-scale modeling with localized enrichment based on discrete microscale and nanoscale methods. The 'handshake' of field variables to ensure continuity at the interface between the discrete and the continuum regions is particularly important and a significant challenge in such hybrid methods [18].

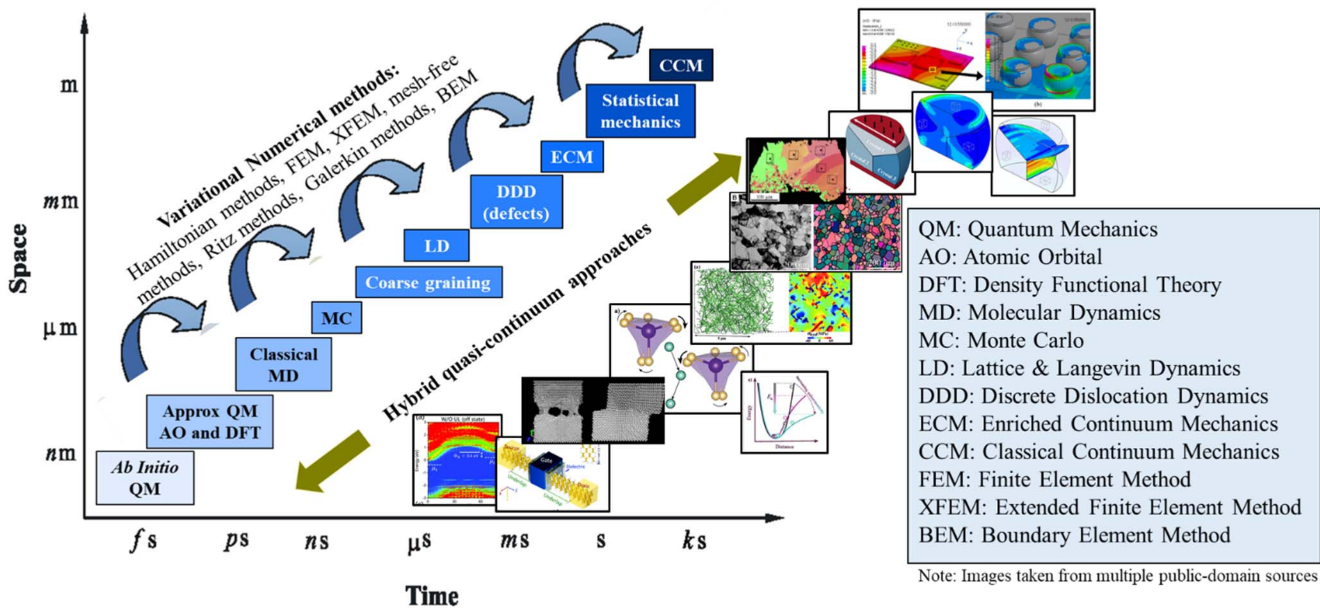

Figure 14. Hierarchical modeling and simulation map, spanning many levels of length scales and time scales

Challenges and Potential Solutions

While multiscale methods have made steady advances in the computational research community, much work is still needed to integrate them seamlessly across length scales in commercial tools and to make them widely available and readily accessible in user-friendly formats. Some of the steps discussed above are further along in terms of commercial tool availability, while some others need significant additional work. As examples, the ECM methods still have rudimentary capabilities in commercial tools and need far more widespread capability.

As heterogeneous integration continues to drive up system complexity and as advancing semiconductor nodes continue to drive down length scales, the complexity of the necessary multiphysics modeling across extensive length scales and time scales will continue to challenge available computing speed. Continuing innovations will be needed in massively parallel computing, hierarchical compact modeling solutions and in quantum computing technologies.

Additional challenges will come from:

- ever-spiraling demands in multi-physics input data descriptions
- defining and measuring material input properties at extremely small length scales
- model validation
- Advanced AR/VR-assisted interactive, user-friendly GUI methods for defining complex model architecture

The goals envisioned for multiscale modeling and simulation will require organized collaborative efforts to leverage the expertise and resources of: (i) the computational research community, (ii) commercial computational tool developers, (iii) high-performance computing ecosystem builders, (iv) the computational user community, (v) the modeling standards community, and (vi) the relevant experimental community (for materials characterization and model validation). Therefore, significant focused industry-government global partnerships and initiatives are needed for the development of sophisticated (multi-physics and multi-scale) modeling capabilities, efficient numerical algorithms and suitable simulation ecosystems.

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3.6 AI/Machine Learning

Current State of the Art and Challenges

Design-on-simulation (DoS) technology has been widely used in many new packaging developments, but it has encountered some challenges in ensuring simulation results. In recent years, AI/machine learning has been applied to many application domains, and some researchers in the field of electronics packaging have also begun to conduct related research [1-3], that tries to combine AI/machine learning and finite element simulation to estimate the reliability or warpage of the package structure. This state-of-the-art AI-assisted design-on-simulation technology can ensure that the prediction results are within an accurate range.

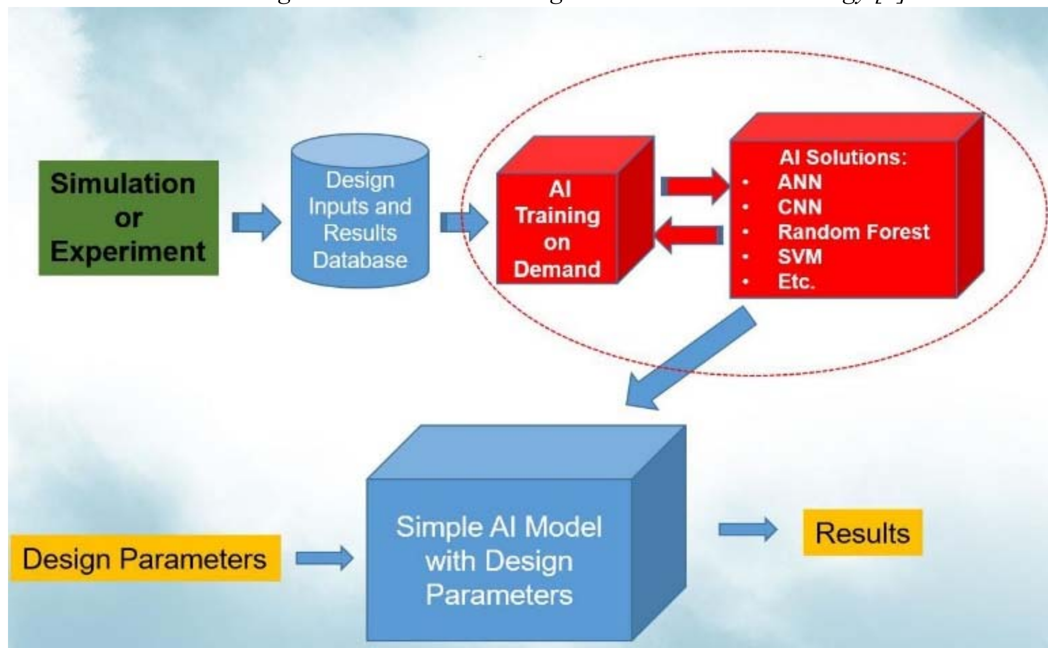
For electronics packaging structures, many design parameters will affect the reliability performance; using experimental results, such as accelerated thermal cycling testing, to obtain the reliability result will take a considerable amount of time. Therefore, how to shorten the design time becomes a critical issue for new electronics packaging structure development. The packaging industry has introduced finite element-based design-on-simulation technology to reduce the number of experiments and shorten the product design cycle. In order to ensure the quality of simulation analysis, researchers must have good domain knowledge, strong mechanics theory, and an FEM background. However, no matter what theories and solving procedures are applied to design simulation, the results of finite element simulations will inevitably depend on the mesh size, and there is no guideline to help researchers address this issue. In fact, the results of simulation analysis are highly dependent on the individual researchers, and the analysis results between them are usually inconsistent. Recently developed AI-assisted design-on-simulation technology can provide a feasible solution to overcome this problem and deliver consistent predictions. The use of machine learning to predict mechanical behaviors is a better way to obtain a reliable result, optimize EP structures and meet the time-to-market demand.

Machine learning [4-8] involves the use of AI theory combined with big data to guide computers for training and learning, with the final goal of developing a prediction model to help researchers make decisions. Machine learning can be applied for regression or classification models using either supervised or unsupervised learning. For electronics packaging design, e.g. reliability and warpage prediction, because the input datasets die thickness, solder pad diameter, buffer layer thickness, etc. are labeled, the learning algorithm for predicting the reliability is considered supervised and belongs to a regression-type model. Several machine learning algorithms are suitable for AI-assisted DoS technology, such as artificial neural network (ANN), support vector regression (SVR), K-nearest neighbor (KNN), kernel ridge regression (KRR), recurrent neural network (RNN), random forest (RF), Gaussian Progress Regression (GPR), Polynomial Regression (PR) and convolutional neural network (CNN). Taking solder joint reliability prediction as an example, the aim of the AI model is to learn and establish a regression model for the relationship between packaging geometry (input) and reliability life cycle (output) results. After the AI training is completed for selected materials, the engineer only needs to input geometry data of each component of the package, and the reliability life-cycle result can be obtained immediately. However, machine learning requires big data for training; the main challenge of this AI-assisted DoS technology is the lack of data, e.g., reliability life cycles of packages. There is not much experimental data available to researchers, which makes it difficult to apply the AI-assisted DoS technology.

Potential Solutions

Validation is a very important procedure for design-on-simulation technology. In order to achieve the goal of AI-assisted DoS, a series of verifications are required, such as basic mechanics theory, materials properties, critical mesh size and standard finite element simulation procedures, which should be verified through experiments before generating a large input/output database for AI, and this work should be completed by experts in these fields. For reliability prediction, if the simulation results can accurately and continuously match the experiment results, the experimental work such as accelerated thermal cycling test can be replaced by this validated finite element simulation process and used to create a large database for AI training to obtain an accurate AI model for reliability/warpage prediction. Once we obtain the final AI model, for a new packaging with the same type of structure, one can simply input the packaging geometry, and the reliability life cycle can be obtained immediately. Figure 15 illustrates this procedure. After AI training, a simple model can be obtained, which contains the relationship between design parameters and results. Engineers only need to enter the design parameters, such as chip size, chip thickness, solder ball diameter, etc., and the reliability results can be obtained immediately. AI/machine learning is a powerful tool for electronic packaging design, but, it requires a reliable database to make correct predictions.

Figure 15: AI-assisted Design-on-Simulation Technology [9]



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3.7 System level simulation

Current State of the Art and Challenges

Product development, such as for an electronic control module, demands rolling out an effective and efficient system design in a short time span and at reduced cost in the face 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 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 influences 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 Experiment (Virtual DoE) is an automated simulation methodology wherein the design space is composed of the range of properties for particular materials that are available in the market. A suitable model is considered where the range of the properties to be evaluated is defined as a 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 property for the components in a timely and cost-effective manner.

In order to predict quantitatively the stress state of design elements, 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 materials 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 of 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 into thermal simulation to obtain the temperature distribution. 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 module under real working conditions is performed. Sub-modeling techniques allow a quantitive estimate of the stress state in a design element. That enables a risk assessment for different failure modes.

Potential Solutions

In recent years there is an upward trend in the usage of microelectronic components in almost all industry sectors. 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 a smart electronic systems seems to be the way forward. To enable 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 packaging 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 Experiment (VDoE) is a potential technique that from one perspective allows pre-selection of materials for the designed system. Ultimately this 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 and economic analysis aids 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. The Virtual DoE [5] technique allows 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 [3,6-9]. This concept is demonstrated in the example described in the following section. The Virtual DoE technique is used to select molding compound for an IC package. The important properties of e.g. molding compound which influence the stress state in 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 availability in the market. Based on the chosen design plan, test cases/data points are generated. The results of the simulation which gives the mechanical response of the electronic control module (or smart system) is used as input for regression analysis. A response surface is generated utilizing a quadratic model which considers the main parameter effect as well as the cross-interaction effects.

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3.8 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: "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]. Thereby, the materials 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 return determine the properties. Due to the trend of ongoing miniaturization, size effects are to 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 – as, for example, hardening of metals during plastic deformation is noticeably different when diverging from bulk behavior 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.

So 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 the 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 properties, as they are especially important for e.g. 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), so they have to be characterized (only on very rare occasions do manufactures 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 as a seamless zooming over the length scales and across physical domains is just about visible on the horizon, there are a lot of challenges to be addressed with respect to materials characterization.

Above all, multi-scale and multi-field modeling paradigms (as highlighted in the previous sections) must be paralleled 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 accounting for 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 materials 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 have. This is a particular challenge for interface properties, and 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 in view of system simulation tools as well as 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 materials 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 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 that include 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 those properties and degradation under accelerated stress testing conditions (vibration etc.). For the fracture mechanics characterization of interfaces [10,11,12], subcritical [13] mixed mode crack propagation data is urgently required, with at least several key descriptors, and all of 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].

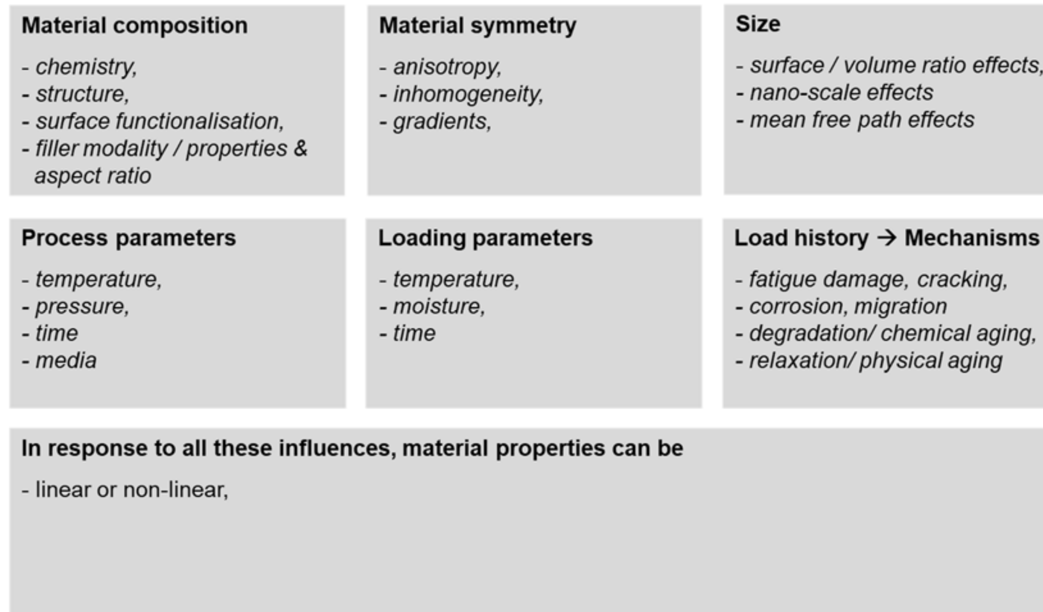

Figure 16: Materials property dependencies on various influences. For engineering purposes the materials have to be characterized to furnish relevant data for simulation input.

From the text and Figure 16 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, with meaningful accelerated stress testing paradigms as well as 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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4.0 Applications

4.1 MEMS & Sensors

Current State of the Art

The modern MEMS world includes many classes of products, such as inertial, optical, chemical, bio, sound [1]. The large variety of products and applications implies the combined use of many physical principles. The complexity of modern MEMS, or better microsystems, in turn implies that modeling and simulation is a fundamental step in the whole process that goes from the first design ideas to the control of production and monitoring and solution of reliability issues. This is the reason why the fast development of microsystems and their widespread diffusion has pushed the formulation of more and more realistic and efficient simulation tools.

High fidelity and efficiency, i.e. reduced computing time, are contrasting needs that can only be satisfied by making use of specific strategies. These have always been put in place by well-informed microsystems designers, e.g. decoupling the various simulations as much as possible, selecting in a clever way the right model and reducing time-dependent simulations as much as possible.

Now various commercial tools exist which enable realistic modeling and simulation, also taking into account many nonlinear effects. Nevertheless, it is not always possible to obtain good results in a reasonable amount of time and in many situations old-style decoupling and smart strategies must be followed by the designers. Design for reliability is a basic principle in microsystems design but the current state of the art in modeling and simulation for MEMS does not always allow for a holistic approach, including e.g. in a unified formulation, models used for in-service conditions and models used for reliability. The same happens if we consider the single sensors and the whole microsystem including ASIC and package.

Challenges

Challenges in modeling and simulation for MEMS are strictly related to the major trends that can be recognized in the expansion of the MEMS world. We list here five clear trends.

Miniaturization, which was the main trend for MEMS in the first phase of their existence, is still important for many applications, in particular for consumer and biomedical markets. Miniaturization is also driven by the need to reduce cost and power consumption.

Increased complexity, arising from the number of physical phenomena that can be coupled in a microsystem, from the integration of many sensors and actuators in a single device and of many microsystems in a more complex device.

New materials, which are being introduced in MEMS, such as piezoelectric materials for sensing and actuation, are now a reality in many products.

New fabrication processes. Microsystems designers have always been constrained by the strict rules of lithography and its mainly planar character; now new fabrication processes are being studied and introduced for industrial products, which also combine additive manufacturing for some steps of the production. These new processes will allow for new geometries and more versatile devices.

Pre-treatment of sensed data. Thanks to miniaturization and to reduced power consumption, it is now possible to design devices which not only sense and transmit the sensed quantity, but also pre-elaborate the sensed data, by means of on-board algorithms and also based on machine learning.

The trends above represent new challenges for modeling and simulation of microsystems:

Miniaturization means an increased importance of surface effects and in many cases the need to cope with nonlinear effects which were disregarded in the first generation of MEMS [2].

Increased complexity implies an increased number of coupled physics which in turn means large scale simulations with an enormous number of degrees of freedom if a high-fidelity model or digital twin must be obtained.

New materials imply new and more complex constitutive behaviors, possibly multi-physics, as in the case of piezoelectric materials with a new class of nonlinearities coming from the material itself.

New fabrication processes call for new modeling and simulation tools, such as in the case of additive-manufactured devices, which can help designers in studying the effects of various fabrications steps.

The pre-treatment of data needs very fast, real-time simulators that can be run by on-board processing units.

New trends are pushing for the creation of new classes of products for new applications. Let us consider as meaningful examples, micro-mirrors, micro-speakers and piezo-micro-ultrasonic-transducers (PMUT).

Micro-mirrors with piezoelectric actuation are now devices on the market. Modeling and simulation in this case include high complexity at the constitutive level, the ability to simulate high angles of mirror rotations, the necessity to carefully estimate fluid-structure interaction for mirrors packaged in air, and the careful examination of reliability issues linked to fatigue in the presence of humidity and high local temperatures.

Micro-speakers are a new class of microsystems that can revolutionize the earphone market. They can be fabricated with piezoelectric actuation. Modeling and simulation for micro-speakers need the careful study of the vibration of the device in a wide range of frequencies, interacting with the surrounding air, in various conditions. Possible thermo-acoustic effects should be considered in the proximity of the vibrating membrane and a careful study of existing air-gaps should be performed. In addition, the total harmonic distortion (THD) of the acoustic signal should be evaluated; this implies the inclusion in the models of many possible sources of nonlinearities.

PMUT have modeling and simulation features similar to those of micro-speakers. In addition, since they are often used in arrays, the issue of cross-talk among membranes is relevant and must be included in the simulation [3].

From the above-selected trends and challenges, it emerges that modeling and simulation for MEMS should be more and more multi-physics, should include more advanced material behaviors, and should be able to realistically reproduce a wide variety of nonlinearities. Moreover, the creation of digital twins for every new MEMS device is now considered a fundamental step to reach the goal of high fidelity simulation for the whole microsystem.

Potential Solutions

Potential solutions to the challenges listed in the previous paragraphs are coming from a combination of strategies that are now reaching high efficiency and from new approaches that are emerging in the world of scientific computing.

- Multi-physics modeling and simulation can be performed in efficient ways due to the adoption of domain decomposition strategies, as shown in [4], also in the presence of highly nonlinear phenomena [5], possibly inserted in multi-scale formulations.
- For many microsystems it is possible to adopt highly efficient Model Order Reduction (MOR) strategies [6]. New trends in MOR for MEMS can be found in [7,8].
- Structural and topology optimization are now powerful tools for the fast design of MEMS; a recent example can be found in [9].
- The formulation of a digital twin for MEMS devices is an overarching goal for modeling and simulation applied to microsystems. MOR strategies combined with deep learning are now emerging that could result in extremely efficient simulation tools, which could enable real-time computing.
- The wide and fast developing world of deep learning is also important for the introduction of on-board computing capabilities in MEMS and for the construction of multi-physics models useful e.g. for materials characterization [10].

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4.2 Manufacturing Processes

The manufacturing processes used to create the packages that protect and interconnect chips (or chiplets) are seeing significant changes in recent years due to a drive for smaller and more powerful chips. Innovations in front-end wafer manufacturing technologies (deposition, etching, etc) and back-end processes (bumping, wire-bonding, encapsulation, etc) are driving quality for advanced packaging. For example, wafer level packaging has become one of the fastest growing advanced packaging technologies, where novel bumping, through-silicon vias, redistribution layers, fan-out, and other techniques are contributing to small-form-factor chips that have powerful, high-speed functionality. These leading-edge packaging technologies are also driving advanced packaging technologies for power semiconductor devices (SiC, GaN) where there is a move away from traditional wire-bonding (high parasitics, low manufacturing tolerances, etc) towards novel die attach materials such as sintered silver and flip-chip interconnections with advanced embedded cooling technologies. For power devices, this benefits power efficiency and supports lower volume and weight for power modules.

Current state of the Art and Challenges

The use of modeling and simulation techniques to predict the performance of advanced packaging processes in terms of the resulting quality of the manufactured package is a key requirement, as poor quality manufacturing processes will significantly degrade performance (electrical, thermal, mechanical) of the assembled chips and subsequently the reliability of the electronic packages and system. Physics-based models, numerical optimization, stochastic techniques, and recently machine learning has been used to predict optimal process conditions to ensure that manufacturing processes meet the requirements for quality. At the chip-level, this supports design rules and associated process design kits (PDKs). At the package level, similar approaches are being adopted to support the design rules for packaging and assembly and associated Assembly Design Kits (ADKs).

Manufacturing processes for packaging at the wafer-level and at board assembly level are highly multi-physics and these processes result in thermo-mechanical and shrinkage stresses. Also poor manufacturing process conditions can result in poor-quality fabrication that will impact subsequent reliability. New manufacturing processes (for example, 3D-printing) require multi-physics models that can predict the evolving stresses that form in the fabricated part and its overall quality in terms of geometry and tolerances. Such models can be used to predict manufacturing process capabilities and tolerances. An example of developments in process models for 3D printing is detailed in Figure 17, where 3D-ink-jet printing is being used to print both conductive and non-conductive inks, and infra-red radiation is used to cure the materials.

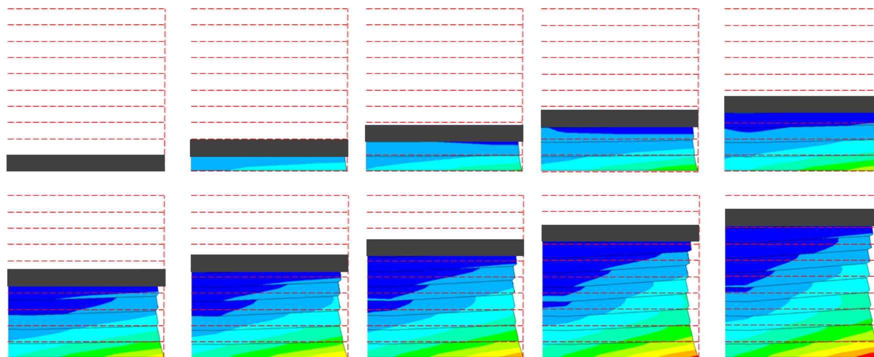

Figure 17: Evolving stress and deformation in 3D-printing process (1)

Potential Solutions

Modeling and simulation developments for manufacturing processes to address the above challenges require (i) detailed integration between state-of-the-art metrology techniques with modeling and simulation to ensure accurate data for modeling (cure kinetics, solidification of metals, etc); (ii) mapping simulation results from process modeling to subsequent electrical, thermal, mechanical and physics-of-failure reliability predictions; and (iii) merging machine learning together with physics-based tools and sensor data within the manufacturing system to develop real-time model-predictive control techniques for each manufacturing process.

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4.3 Composite Materials

Particulate composites are a frequently used material in heterogenous electronic systems, especially as a thermal interface material (TIM). TIM is used as a space-filler between the chip (which usually generates heat that is unevenly spread between components in the chip) and a heat spreader, with the aim of improving the conduction of heat. Often the filler and the matrix consist of combinations such as Silicone/Alumina, Silver/Silicone, Silicone/Epoxy, ZnS/Diamond, etc. Optimizing the micro-attributes of the TIM, such as size distribution of the particles, packing fraction, and the optimal combination of the particle type itself, is a non-trivial task in an experimental as well as in a computational setting. The optimal thermo-mechanical features being sought in an ideal TIM are high thermal conductivity (k_{eff}), low elastic modulus (E_{eff}) and a low viscosity (η_{eff}), which allows for better performance in the primary function, long-term reliability of the packaging, and convenience in assembling. These three properties are closely interlinked, meaning that one cannot arbitrarily vary one without significantly affecting the others and thereby reducing the performance of the material. Therefore, designing the microstructure of these materials for enhanced thermal transport necessitates a considerable research effort.

There is currently no firmly established procedure in formulating the optimal filler combinations applicable for a given use case. The pathway for developing new TIMs is often trial-and-error based, requiring significant consumption of time, effort, and resources. Therefore, the ability to model and simulate the systems and establish data-based procedures is necessary in concocting superior fillers. The typical particle size in these particulate systems demands a higher spatial scale of modeling, falling into the category of mesoscopic systems, which typically deal with the behavior of properties of matter within the nm-µm range.

Computational Aspects

The computational approach for modeling these systems can be broadly divided into three phases:

1. Generating the arrangement of particles (random/preferred)
2. Selecting the theoretical basis for modeling thermal conductance, elastic modulus, and viscosity
3. Optimizing the performance of the algorithms

1. Generating the arrangement of particles (random/preferred)

Simulating the arrangement of filler particles in the system is typically done in one of two ways:

A. **Collective arrangement of particles**: A predefined system of particles with known size distributions and positions within the cell being updated each time which results in higher packing factors being achieved. However, this requires expensive computational effort with an increasing number of particles. This method also requires an additional computation of particle-particle interactions. {*Lubachevski-Stillinger algorithm*[1], *Kansal-Torquato-Stillinger algorithm*[2], *collective random walk*[3,4], *combined static/dynamic approach*[5,6], and *distinct element method*[7,8]}

B. **Sequential Addition of particles**: Particles are generated one after the other in a predetermined procedure allowing for different particles with a distributed range of sizes and types with non-overlapping regions to co-exist. This method allows faster generation of systems but does not allow higher packing fractions to be achieved. {*Random drop*[9], *drop-fall-shake*[10], *random walk/contact algorithms*[11,12]}

The particles thus generated are spherical and represent particulates in a TIM setting. The systems currently developed seem to have no periodicity. From either method the final structure that is derived is more critical to the final result compared to the initial setup of particles or transient systems; therefore there is a tendency to use the sequential method.

2. The theoretical basis for modeling

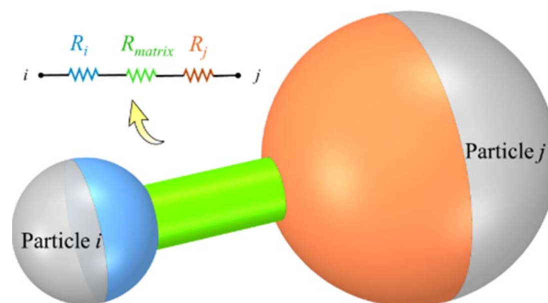

Figure 18: Thermal Resistor Model for thermal exchange among particles (Adapted from ref. [13])

Figure 18 details a model for the thermal conductance of the material, which is usually modeled with the use of thermal resistors, effectively replacing the spherical system with a network of cylinders with variable radii and lengths connecting each nearby particle with a cutoff based on the spatial arrangement and distance. This follows the work by Batchelor et al [14] and further improved by Dan et al [15] and by Subbarayan et al [16]. In newer models, allowances are made for parallel conduction pathways where heat from particle A to particle B could be transported directly or indirectly via one or more other particles. The vertical boundaries are considered adiabatic with no thermal connection to periodic images.

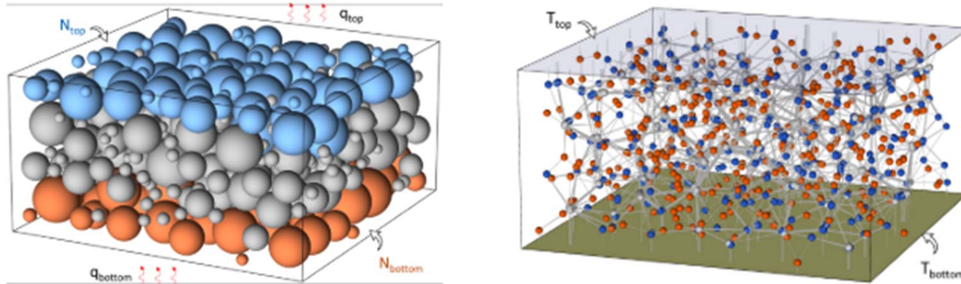

*Figure 19: **Left**: A system with adiabatic sidewalls (non-periodic) connected to the bottom (heat in) and top (heat out) surfaces thermally; **Right**: The same system with the interparticle network with lines, particles and horizontal boundaries representing pathways available for heat transfer (Adapted from ref. [13])*

Once the thermal resistances between particles are determined, this interparticle network (see Figure 19) of resistors is a global network of thermal resistors. The particles become nodes where each could be connected to several others or left isolated depending on the parameterization values chosen for a system. Using prescribed boundary conditions for upper and lower surfaces, the temperature at each node is determined which is then used to calculate the effective thermal conductivity.

For the determination of the effective elastic modulus of the system, the same framework used to determine the thermal transport can be used based on the works of Vaitheeswaran et al [16] where the applied force flux is supported by the filler particulates. The particles hence become a network of springs behaving under the conditions imposed by connectivity to each other. The system is assumed to be uniaxially loaded under the assumption that the sidewalls are stationary. The heat and force transfer of the system is assumed to be analogous, allowing for the use of modified Batchelor and O'Brien's analytical solutions to solve for the stiffness of each spring and thus allowing the calculation of the effective elastic modulus of the system [14].

For the prediction of effective viscosity of the system, the work involving mono-disperse systems are expanded onto polydisperse systems based on the works of Dorr et al [17]. The modified Quemada viscosity relation [18] which models the viscosity in monodisperse systems is used as the basis, where the first and second coefficients are derived analytically from the Stokes equation for 3D dilatational flow in a suspension of randomly located spheres and for the absence of Brownian motion by the works of Batchelor and Green respectively [19].

Improvements for the Future

While the up-to-date literature indicates a progressive improvement in the size of the systems being modeled and the quality of the data from modeling, there is a considerable area for improvement in building a consensus among the various models and algorithms being developed. Currently there seems to be no feed-forward path for data from atomistic scale modeling to the mesoscopic level simulation used in present work; rather, it relies instead on a mechanistic parameterization based on available empirical data, which limits the transferability of the results across various TIMs in use. Additionally, there is room for improvement in the inclusion of other parameters in the system as well as the fine-tuning of ones already in use [13].

The use of genetic algorithms in the modeling process as seen in the recent work of Su et al seems to be promising in integrating machine learning with the current numerical systems with the ability to model higher packing fractions within reasonable computational efforts [20].

The algorithms currently found in literature do not appear to be parallelized which would enable the utilization of massively parallel computing systems. Parallelization of the numerical systems is essential in being used for the generation of simulation systems with denser packing and higher volume fractions. This would also enable the creation of an open database where the components of fillers and matrix could become readily available for the materials designers for the electronics packaging industry. The goal would be to have access to these algorithms,

either as open or commercial ventures, eliminating the need for expensive and time-consuming internal development of software packages used for the simulations.

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4.4 Reliability and Prognostics

Current State of the Art and 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 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 20.

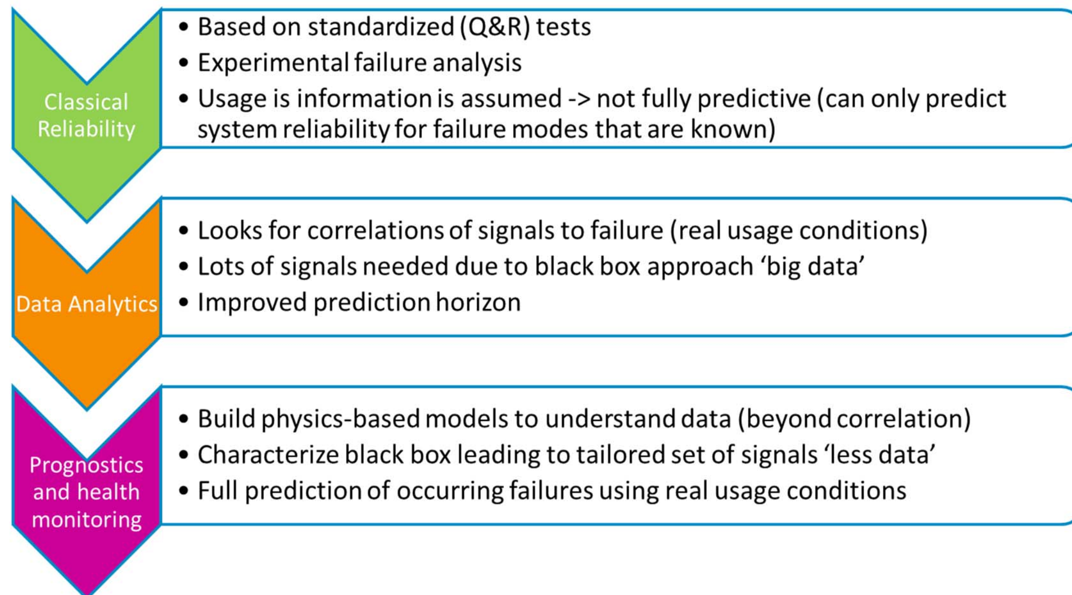

Figure 20: From standardized test-to-pass testing towards prognostics-based performance measurements.

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 adaptation to the specific new PoF situation, see also Figure 20 [5-7]. 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 from huge data sets (based on past qualification and reliability tests) will also provide knowledge to support reliability modeling [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- and 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:

- 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 (including '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 21, 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, virtual 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

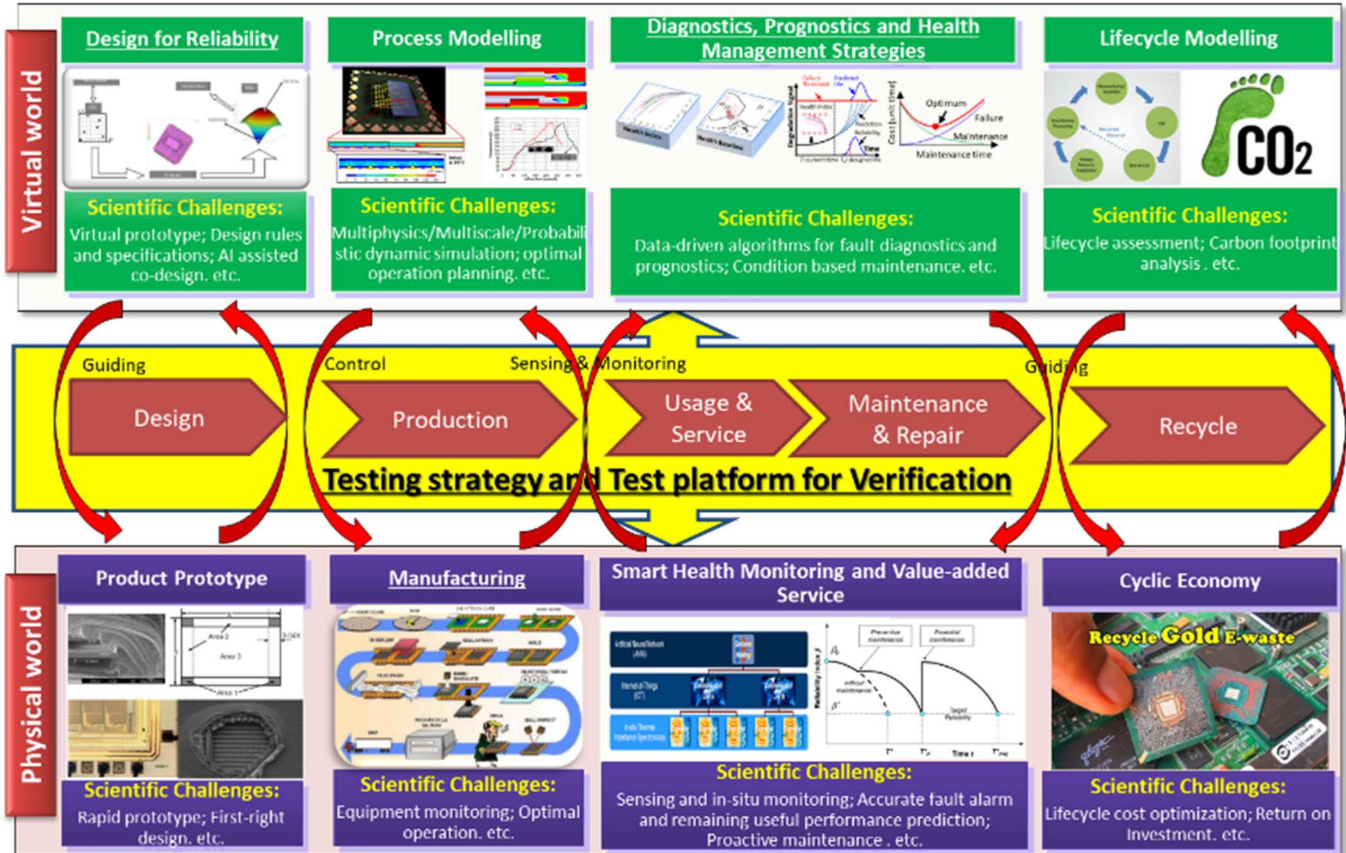

Figure 21: Digital twin for electronic components and modules (Source: G.Q. Zhang & Jiajie Fan)

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. This horizon is listed in Table 2.

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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)

4.5: Digital Twins

What is the Digital Twin?

We define a digital twin as the instantiated model (numerical, analytical, hybrid) of a specific asset or device, which is deployed (in the cloud or on an edge device) and connected to the physical device (see Figure 22). The connection may be established through sensors installed at the device or other sources collecting specific information (e.g. control units, weather forecasts, devices nearby, etc.), delivering a continuous data stream fed into the model or as boundary condition or as reference value.

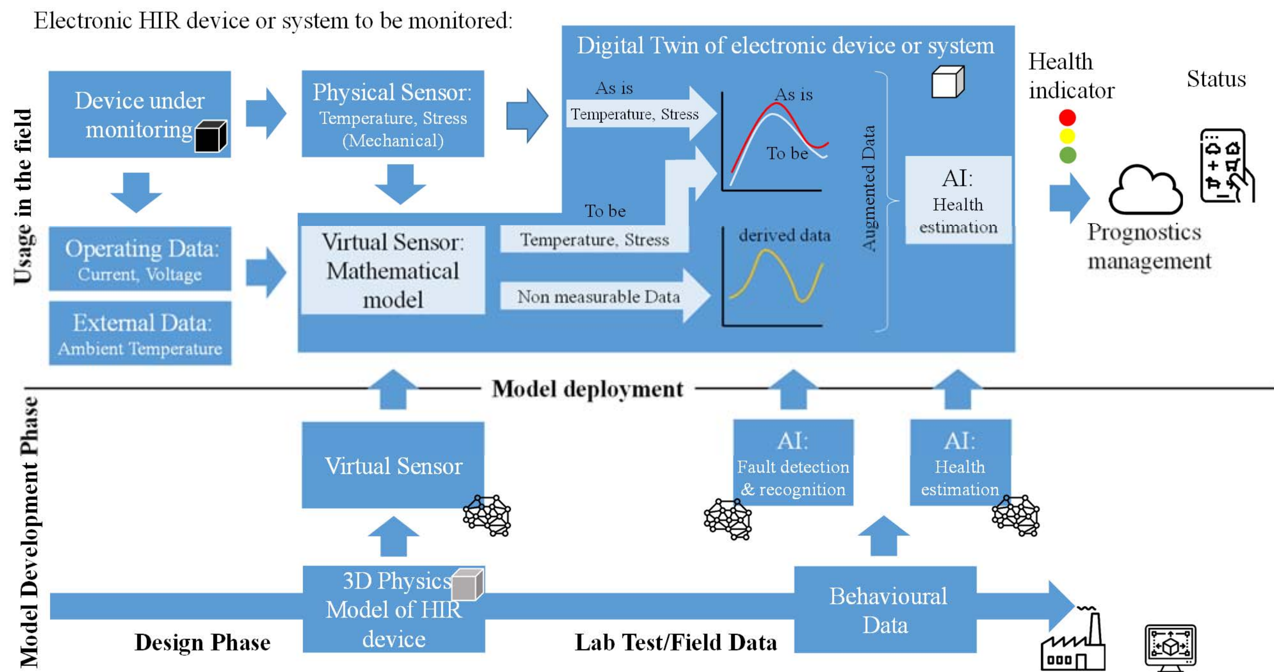

Figure 22. The digital twin concept applied for prognostic health management of electronic devices and systems

The digital twin is a powerful methodology for future, complex electronic devices and systems [1]. Below, we listed some of the benefits:

- Exploration of information at positions where the placement of physical sensors is impossible (due to geometrical restrictions (e.g. stresses in solder joints), hazardous conditions (e.g. aggressive or abrasive media))
- A digital twin enables virtual sensors in many different locations that allow getting a full temperature, stress or strain field of the monitored system.
- Using a digital twin, we have capabilities to evaluate a non-measurable quantity (e.g. accumulated plastic strain in solder).
- Using virtual sensors, we can reduce the number of physical sensors or replace expensive physical sensors with low-cost sensors and virtual sensors.

There are already best-practice examples of how the digital twin has been implemented:

- **New business models**: operation as a service. Here in this example, a virtual torque sensor for a downhole Pump for Oil and Gas Applications: Determination of critical operation conditions to prevent pump failure [2].
- **Optimization of process control**: Inductive hardening: online and on-site computing of influence of process parameters on resulting temperature distribution to improve hardening result, scrap reduction and process speed up [3].
- **Degradation monitoring at the IC device level**: example of the degradation of IC devices supported by an AI/ML method. Based on in-situ monitoring, it is possible to monitor vital parameters of the IC and its environmental stress based on a physics of failure model to estimate the time to failure [4].
- **In-situ degradation monitoring**: implementation of the virtual sensor using a surrogate model to monitor delamination of the die attach during reliability test [5]. The data is generated by piezoresistive sensors to monitor the stress state during accelerated test. In order to estimate crack formation, a virtual sensor in the layer of the die attach has been modeled using a surrogate model.

Current State of the Art

There are already available methods that allow implementation of the digital twin (see Figure 23) either in the cloud or on edge devices. In essence, it is a model or a set of models that uses real-world data for simulations to predict how a product or process will perform. It can use any sort of model that is a sufficiently accurate representation of the physical object.

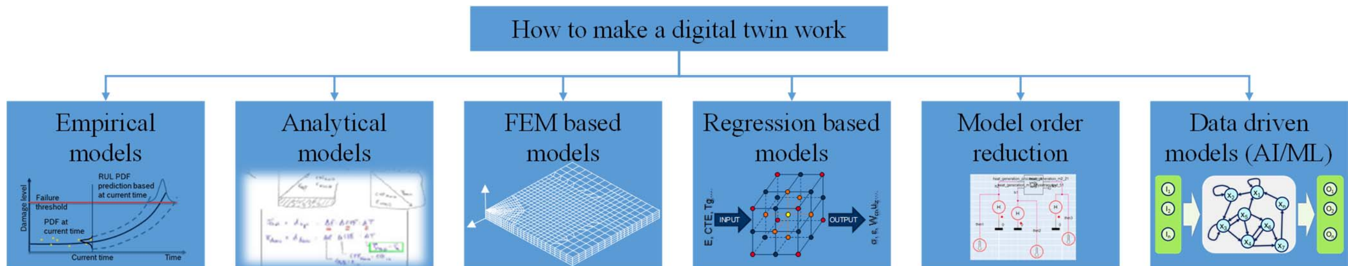

Figure 23. Available methods to create a digital twin

The following models are in use:

- Empirical models. They are built based on observations from measurements/experiments. For example, cracks have been found to be generated and propagated in thermal-cycle tests due to low-cycle material fatigue. The Coffin-Manson relation describes this effect by fitting two empirical constants. To avoid some limitations, more accurate/complex models were developed such as Norris-Landzberg, Engelmaier and others.
- Analytical models. They are used in situations where the behavior is dominantly controlled by effects for whose description mathematical relations are available to output the desired physical parameter. For example, a mathematical model is used to connect the driving profile to the IGBT power dissipation.
- Numerical models. They use computational methods like FEM, Molecular Dynamics, Computational Fluid Dynamics etc. to reach higher accuracy even for complex situations and systems. Often, the simulation requires substantial time (several minutes, up to many hours) even with high-speed computation units. This might affect the applicability for real-time decisions.
- In some applications, compact models of the physics-based approaches can be built based on the full-scale numerical models.
  - Model Order Reduction – efficient numerical simulation – “solves in seconds vs. hours”. It reduces the full model to a desired part of the system (e.g. node, element) to calculate the output, using different projection methods, such as:
    - Iterative Rational Krylov Algorithm
    - Balanced Truncation (BT)
  - Statistics (regression-based models) are used to describe the entire response surface based on specific parameter ranges. It uses the input and the output of the full model simulation.
  - Metamodels or surrogate models that mimic the behavior of the simulation model as closely as possible while being computationally fast to evaluate. These use methods such as Artificial Intelligence (AI) and Machine Learning (ML).
- Data driven-based models are purely data-driven, built only on measurement data. They use methods such as AI and ML.

Challenges

In real product applications, specifically in the microelectronics industry, failures occur due to temperature-induced loads. As the materials involved typically have different coefficients of thermal expansion, thermal changes lead to stress accumulation, which causes the failure. Most materials show a temperature dependence and some of them also time dependence in their behavior. Therefore, the typical temperature-induced stress/strain evolution is highly non-linear. As of now, there is no generally accepted method for considering such effects in compact models, which are seen as a key enabler for digital twins that can be implemented at the edge, i.e., into the electronic system itself as the basis for the necessary health assessment and management. This is why research is needed to develop such compact digital twins by focusing on the following four fields:

Temperature dependency: This is the first challenge to be addressed. Although it seems to be relatively easy, there is still some effort required to finalize the development and deployment of digital twins that capture temperature dependency of materials in final micro-electronic products.

Time dependency: This is specifically important for the digital twins of electronic devices and systems deployed in the field, where the specifically time-dependent effects, such as relaxation, aging, corrosion, and abrasion, lead to major wear-out related failures.

Non-linear effects: One of the possible solutions for considering nonlinear effects is to build the compact digital twins by using artificial intelligence and machine learning methods. There have already been first attempts made to

capture complex behavior of electronic devices and modules and simulate using the compact model's non-linear behavior based on AI and ML and a lot of research work is aiming at fully using this potential of AI/ML. As part of these efforts, the definition of the requirements regarding the training and validation should lead to a commonly accepted standard.

Multi-field/multi-domain requirements: Specifically, for complex systems like complete electronic control units (ECU), the evaluation of the damage is very challenging. Traditionally, multi-domain simulations using coupled electro, thermal, and thermo-mechanical simulation have been used during the ECU development. In addition, sub-modeling techniques have been used to evaluate the stress for the small (but essential) design elements such as the solder joint. A similar approach must be developed as fully automated tools used locally on the device or ECU level (as edge computing) and combined with more complex numerical models that can be executed in the cloud.

Multi-scale effect: Multi-scale effects are caused by the very different length scales in semiconductor technologies, e.g. related to production process of semiconductor and microelectronics devices. Here, we also require new approaches to integrate simulation approaches using e.g. molecular modeling, geometry-based modeling such as FEM, including behavioral modeling which allows the model to transfer the load from the system level (m) to atom levels (nm and below).

Further standardization of the **exchange format** for model exchange, such as function mock-up interface (FMI) and function mock-up unit (FMU). Exchange of the data and models should be as easy as in the case of ASCI (txt) or CAD data.

Deployment: During real operation, there is a lot of data generated. In the case of the digital twin, the information will be multiplied, as we will generate data not only for the real sensors, but for virtual sensors as well. This enormous volume of data cannot be transferred to the cloud. Transferring all this information is not desirable; however, there must be a HW/SW solution which will allow for edge computing. In this case, the data generated during active operation of electronic devices or modules will be pre-evaluated locally, and only the required information will finally be transferred to the cloud. Execution of the simulation models at both sites, i.e., at the edge devices and in the cloud, must be done autonomously and be fully automatic. Here, further cooperation between academia, industry, and SW developers is required.

Life cycle management of the digital twin: During operation, the physical asset may be subject to willingly induced alterations (e.g. software updates, exchange of spare parts, etc.). These alterations need to be reflected in the digital twin. Additionally, there may be improvements made on the models applied. These could be updated; nevertheless, the current state of the physical device needs to be stored and correctly represented in any model version. Thus, the versioning, tracking, commissioning, and decommissioning of the models is crucial, which leads to the necessity of a life cycle management plan for the digital twins.

Degradation criteria and performance indicators: we need to get the damage parameters corresponding to the degradation state and avoid potential failure. This degradation criteria and performance indicator should describe the status of the device (e.g. delamination in the package is detected). Compact models should be able to predict specific parameters based on the information about the loading conditions such as power dissipation or ambient temperature. If deviation of one or some parameters appears, a digital twin should be able to estimate if it is caused by e.g. ambient temperature or by deviation caused by degradation. This can be realized by a self-aware twin builder that has implemented functionality for fault detection and recognition.

Interaction of multi-degradation states: during accelerated reliability tests and usage of the devices and the electronics system, material will be exposed to different types of aging. This might lead to a change of the performance and potential degradation of the systems. As a consequence, that material degradation can lead to other failure modes. A self-aware digital twin should allow for such possibilities.

Process modeling: how to consider residual stress in the digital twin and device or system-specific characteristics. The challenge is how to implement variability caused by materials properties, geometry variations, etc. in the digital twin. Based on that detailed model, we may significantly improve the performance of the digital twin itself including degradation prediction.

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Table 3: Anticipated Solutions

DIGITAL TWIN ROADMAP		
Short term goals (<5Y)	**Middle term goals (10Y)**	**Long term goals (15+Y)**
Digital twins of electronic devices and systems introduced in first products, mainly based on linear analysis, such as temperature, vibration	Digital twins are capable to capture temperature dependent behavior	Digital twin allows damage detection and trigger resilient actions to assure availability of electronic devices and application
Digital twins considering single manufacturing process available (e.g. soldering or sintering)	Solution for edge computing that allow to use digital twin on device or sub-system (module) level	Application of digital twin for prognostics and health management of electronic devices and modules
	First successful implementation of digital twins considering non-linear effects using AI/ML based algorithms	Application of digital twin for prognostics and health management of electronic devices and modules
Deployment and edge/cloud time line	Deployment and edge/cloud time line	Deployment and edge/cloud time line

5.0 General Metrics for Modeling and Simulation

Table 4 presents a Modeling and Simulation Metrics for 5, 10 and 15 years ahead, in terms of the accuracy of material model/property, the accuracy of modeling, and effectiveness and efficiency of modeling and simulation.

Table 4. Modeling and Simulation Metrics

Metric	5 years	10 years	15 years
Development Time from Concept to Product	5 years	3 years	18 months
Accuracy of Material Model/Property	>50%	>75%	>90%
Accuracy of Modeling	>50%	>75%	>90%
Effectiveness of Modeling and Simulation	Validated modeling for known failure modes with multi-physics modeling at different levels	Accurate modeling for comprehensive failure modes/mechanisms, with combined multiphysics modeling with multiscale modeling	Accurate and predictive modeling for unknown failure modes/mechanisms, with comprehensive multiphysics modeling combined with multiscale modeling and stochastic modeling
Efficiency of Modeling and Simulation	Simulation tool capable of multiphysics modeling across different domains (chip/package/board/system) mainly based on linear analysis	Simulation tool capable of multiphysics and multiscale modeling across different domains with mixed linear/nonlinear analysis	Simulation tool capable of multiphysics and multiscale modeling across different domains with fully nonlinear analysis

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