Chapter 14: Modeling and Simulation

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# Table of Contents

1. EXECUTIVE SUMMARY ................................................................. 1
2. SCOPE ......................................................................................... 1
3. STATE OF THE ART, DIFFICULT CHALLENGES, POTENTIAL SOLUTIONS ........................................................................ 2

## CHAPTER 1: HETEROGENEOUS INTEGRATION ROADMAP: OVERVIEW ................................................................. 1

## CHAPTER 2: HIGH PERFORMANCE COMPUTING AND DATA CENTERS ................................................................. 1

## CHAPTER 3: THE INTERNET OF THINGS (IOT) ................................................................................................. 1

## CHAPTER 4: MEDICAL, HEALTH & WEARABLES ................................................................................................. 1

## CHAPTER 5: AUTOMOTIVE ......................................................................................................................... 1

## CHAPTER 6: AEROSPACE AND DEFENSE .................................................................................................... 1

## CHAPTER 7: MOBILE ............................................................................................................................... 1

## CHAPTER 8: SINGLE CHIP AND MULTI CHIP INTEGRATION ........................................................................... 1

## CHAPTER 9: INTEGRATED PHOTONICS .......................................................................................................... 1

## CHAPTER 10: INTEGRATED POWER ELECTRONICS ........................................................................................ 1

## CHAPTER 11: MEMS AND SENSOR INTEGRATION ........................................................................................ 1

## CHAPTER 12: 5G COMMUNICATIONS ........................................................................................................... 1

## CHAPTER 13: CO DESIGN FOR HETEROGENEOUS INTEGRATION ............................................................... 1

## CHAPTER 14: MODELING AND SIMULATION .................................................................................................. 1
  1. EXECUTIVE SUMMARY ................................................................. 1
  2. SCOPE ......................................................................................... 1
  3. STATE OF THE ART, DIFFICULT CHALLENGES, POTENTIAL SOLUTIONS ........................................................................ 2

## CHAPTER 15: MATERIALS AND EMERGING RESEARCH MATERIALS ........................................................................ 1

## CHAPTER 16: EMERGING RESEARCH DEVICES .......................................................................................... 1

## CHAPTER 17: TEST TECHNOLOGY ............................................................................................................... 1

## CHAPTER 18: SUPPLY CHAIN ..................................................................................................................... 1

## CHAPTER 19: SECURITY ............................................................................................................................. 1

## CHAPTER 20: THERMAL ................................................................................................................................ 1

## CHAPTER 21: SIP AND MODULE SYSTEM INTEGRATION .................................................................................. 1

## CHAPTER 22: INTERCONNECTS FOR 2D AND 3D ARCHITECTURES ......................................................................... 1

## CHAPTER 23: WAFER-LEVEL PACKAGING (WLP) .......................................................................................... 1

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Chapter 14: Modeling and Simulation

1. Executive Summary

Design and Modeling and Simulation (M&S) tools are key enabling technologies for Heterogeneous Integrated Electronic Systems that will support product development across the chip-package-board-system domains. This chapter details the key challenges and potential solutions over 5-, 10-, and 15-year horizons, and detail how these tools will support the knowledge base for heterogeneous integrated electronic systems as detailed in figure 1.

![Figure 1: Supporting the Knowledge Base for Heterogeneous Integration](image.png)

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

For example, influences from other physics is assumed in a crude manner (e.g. package thermo-mechanical stress generally assumes a constant temperature profile, where in reality the die electro-thermal behavior and hotspots are transient; and generally ignores detailed 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 for modeling and simulation tools in the following areas:

1. Electrical Analysis
2. Thermo-Mechanical Analysis
3. Mechanical and Multi-Physics Analysis
4. Molecular Modeling
5. Reliability and Prognostics

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

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

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

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

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 physics-based models to support co-design and the knowledge base for heterogeneous integration.

While Moore’s Law economics have come to an end, scaling to advance nodes continues with EUV process 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 & 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. An additional consideration will be differing requirements for different markets – Mobile (consumer smart phones), Data Centers, Mobile Networks, and Automotive.
3.1 Electrical Analysis

Current State of the Art and Requirements/Challenges

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

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

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

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

For printed circuit boards, where the structures are large compared to the wavelength, high-frequency analysis that includes the coupling of the electric field and magnetic field are required. Such analysis requires the use of full-wave 3D field simulators that solve the wave equation derived from Maxwell’s Equations. High-frequency behavior such as transmission line, skin depth, and radiation effects are captured in these simulations. Most commercial tools can export frequency-dependent s-parameter models for the interconnects. These can then be used in SPICE simulators which can handle full-wave s-parameters in both time and frequency domains by creating compact models based on pole-zero and/or state-space modeling. For high-speed channels with serial components, however, simulators with 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, the time of the design and analysis likely does not overlap. The individual (largely independent) tools and methodology for each component level allow a system design to depend on components that are being designed on very different schedules by different teams for non-homogeneous designs. For a logic semiconductor component, the design schedule from concept to logic entry to physical design to tape-out is much longer than a package design schedule, and the packaged semiconductor is likely completed before the printed circuit board design. The silicon team would be redeployed before the printed circuit board design begins and even if co-design could be done, it would at best give a more accurate analysis of the final signal or voltage waveforms with an optimized PCB; it would not improve the semiconductor design or enable an optimization of the design across the package hierarchy since the semiconductor component is already being manufactured. A broad segmented supply chain has developed to support this model of design.

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

To fully exploit the performance capability of 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. This will include co-analysis to enable the simulation of the electrical behavior of this design. The co-analysis can also be used to increase the simulation accuracy of a completed design.

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

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

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

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

**Potential Solutions**

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

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

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

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

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

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

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

The development of co-design and co-analysis methodologies along with the models to facilitate the methodologies creates the opportunity to apply machine learning and deep data analysis to the designs. Deep data techniques will enable design space exploration to accelerate the capability of the designs. A possible timeline would be to use deep data techniques to improve approximation techniques for signal integrity, power integrity, or thermal response in the next five years across the design space of individual components, and in the middle term of five to ten years expand the techniques to approximate response of co-analysis techniques. Independently, the ability to analyze across multiple components can be developed. In the long term, combining the ability to explore the design space for co-analysis and multiple components simultaneously is a goal.

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

References:

3.2 Thermomechanical Modeling

**Current State of the Art and Challenges:** The vast majority of thermal/thermomechanical design rules in electronic design and packaging are based on finite element method (FEM) based simulations post electronic design [1]. Robust thermomechanical models are not present in the electronic design and reliability flows, thus necessitating significant margins from the designers. The power dissipation and power density in future 2D-3D packages is expected to increase and the cross-talk between different functional components of IC packages will further aggravate the thermal management challenges. This will necessitate development of multi-physics simulation tools with closely coupled thermal, mechanical and electrical models to enable iterative simulations and robust design. Such coupled models which 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 packages 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 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.

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

- **Definition of the design space and execution of FEM simulations with combinatorial and probabilistic input parameters spanning geometrical descriptions, material properties and interface/boundary conditions across domains.**
- **Training Data:** Output FEM state distributions and fields (electric field, power density, temperature, stress, strain etc.). Training and validation using an artificial neural network with feedforward deep auto-encoders (DAE).
- **Deployment of the validated DAEs generated to accurately predict the non-linear and statistical behavior of a design with minimum computational and setup overhead.**
One example of such deployment in the thermal domain is by Zhang et al. [4] who apply machine learning to real-time thermal prediction/management and demonstrate improved accuracy, as well as significant runtime overhead reduction.

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

**References**


### 3.3 Mechanical and Multi-Physics

**Current state of the art and challenges**

Stress modeling of heterogeneous systems should contribute to the following (1) design for reliability (stresses as inputs to reliability models) (2) design for yield (stress contribute to development of chip-package-system design rules) (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 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;
- Stresses in through-silicon vias (TSV’s).

At present the majority of stress analysis performed is at the package or board level. Chip-package interaction is becoming more important and die designs now need to consider the stresses imposed on the die from the package.
Hence there is a need for chip-package co-design in terms of package design on the subsequent stress states at the BEOL and FEOL of the die and the impact these will have on the performance of the die.

Modeling and simulation tools have the capability to simulate the mechanical behavior of a package which is subjected to a number of environmental conditions such as temperature, vibration, shock, etc. MCAD Tool vendors provide co-design capabilities that include thermo-mechanical analysis, including effects such as thermally induced stress, and sub-modeling techniques can be used to transfer results from the system (board) level domain to structures at the die level as detailed in figure 5. However, these capabilities do not generally have accurate models for critical failure modes that will be important in 3D heterogeneous systems. Also, there are weak linkages between these MCAD (finite element) tools and EDA tools for electrical analysis to support full chip-package-system co-design [1].

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

Most of the mechanical simulation focuses on the thermal stress due to thermal mismatch only (isothermal condition). The effect of temperature gradient in transient or steady state is not taken into consideration. Moreover, moisture absorption/desorption will also induce additional mechanical stress. For moisture-sensitive materials [2], 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 [3,4] is of critical concern for electronic devices, especially as technologies in microelectronics are going in the direction of scaling from micrometer scale to nanometer scale, and from two dimensions to three dimensions. For electromigration to be analyzed, mass transport, thermal-migration, and mechanical stress-migration must be coupled with electromigration for an accurate prediction.

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 [1] or two-way coupling of the relevant physics. Figure 6 shows the physics domain involved in the multi-physics modeling for a heterogeneous system.
Currently available CMOS technology can already manufacture ICs with feature sizes down to a few nanometers. To assemble the IC into various packages to form heterogeneous systems, one has to deal with integration of geometric dimensions from nano to micron to macro-scales. Due to the huge scale difference, size effects will become essential. These size effects are often related to microstructures and their evolution, various gradient effects (such as chemical, electrical, thermal, and mechanical gradients), and surface effects. In addition, at the atomic level, it is virtually impossible to design a process with deterministic performance. At the macro-level, for design parameters such as material/interface properties, geometric dimensions, process windows, and loading intensities, deviations represented by different statistical characteristics and magnitudes are inevitable. Figure 7 shows the evolution of microstructure of a copper metal line for different technology nodes.

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

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

Potential solutions

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

Accurate materials data and characterisation 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, and there is a lack of consensus on accurate constitutive models used – for example, for non-linear materials such as solders.

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 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.

3.4 Molecular Modeling

Current state of the art and challenges

As feature sizes shrink and IO footprint densities increase, the material issues must address a paradigm shift from bulk properties to direct inter-molecular or inter-atomic interactions. That is, it is realized that as the bulk-to-interface ratio shrinks, more importance must be placed on the molecular or atomistic interfacial properties, which are fundamentally different from the bulk properties. Molecular modeling [1,2] can be employed to help define the differences between the bulk and interfacial properties, and can identify how well specific molecular interfaces interact and how that interaction transforms to create failure. Molecular modeling can be employed at various stages in the life of the interface to inform the developer whether the risk in using a specific material is warranted or to inform the reliability engineer which material/condition combination is at risk. For instance, the question of how the interface structure evolves inherently must address several different questions: a) what is present at initial formation; b) what is present after all the processing steps are finished; c) what is present after low-level condition (stress/temperature) cycling; d) what is present after high-level condition (stress/temperature) cycling. Molecular modeling can be used to define structures present, from both chemical and physical transformations. In addition, molecular modeling allows a prediction of both the strength of a molecular interaction, and also how those interactions may transform under specific temperature, pressure and stress conditions. The basic goal in all molecular/atomistic modeling is the calculation of the energy changes and the accompanying transformations in the...
molecular structure that are responsible for the energy changes. The basic tenet is the belief that it is the evolving structures which describe the evolving interfacial properties.

All molecular modeling packages contain the constitutive equations which represent the atomic, molecular, and crystalline interactions. The packages are separated by the underlying assumptions made: a) quantum level (calculating the energies and resulting spatial interatomic characteristics resulting from atomic wavefunctions); b) molecular (calculating the molecular interactions from generalized atomic interactions found in force fields); and c) mesoscale (calculating higher size order interactions from parameterized molecular groups). The molecularly based mesoscale level is currently evolving; it is becoming popular to scale to higher length and time scales without the expense of larger computation power, which can be very useful when multi-interfaces are considered.

Today, quantum level programs, on a practical level, employ density functional theory (DFT), and 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.

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

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

**Potential Solutions**

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

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

The molecular dynamics and mesoscale areas need better force fields for all metals and their oxidized forms, 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. Force field development will continue to be an ongoing effort.

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

In addition, the link between the atomistic to molecular to mesoscale level needs further defining. On a wider scope, backward and forward scaling is needed between the microscale and molecular (atomic) levels, so that atomistic-molecular-mesoscale-microscale are readily bridged at-will. For instance, if the mesoscale level analysis finds that a certain interface is at risk, the modeler can zoom in to the molecular or atomistic level to define which chemical structure is contributing (crystal, molecular or atomistic level). Length-scale bridging is an area that will not be immediately available, and is expected to be a longer-term issue (within the >10 year time frame).

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


3.5 Reliability and Prognostics

Current state of the art & challenges

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

- Continuous growth in number, complexity, and diversity of the functional features, of the devices and components integrated, and of the technologies and the materials involved in each product;
- Increase in reliability and safety level to be achieved by the products, which will simultaneously and more frequently be deployed to ever harsher environments;
- Decrease in time-to-market and cost per product due to the stronger global competition;
- Higher complexity and depth of the supply chain, raising the risk of hidden quality issues.
With the increasing amount of complexity, it is imperative for the reliability of heterogeneous integrated systems to move from standardized test-to-pass towards prognostics-based performance measurements, see figure 9.

![Figure 9: From standardized test-to-pass testing towards prognostics-based performance measurements.](image)

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

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

While virtual schemes based on numerical simulation are widely used for functional design, they lack a systematic approach when used for reliability assessments. Besides this, lifetime predictions are still based on old standards (MIL, FIDES, Telcordia, etc.) assuming a constant failure rate behaviour [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.

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

Prognostics and health management (PHM) is the next step from condition monitoring; it is not new by itself but needs to be fuelled 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 (incl. ‘smart redundancy’) and alarm management algorithms
- Monitoring test structures and/or monitor procedures (also: using available data) at the component and module level for monitoring temperatures, operating modes, parameter drifts, interconnect degradation etc. – according to the failure Pareto plot
- Identification of early warning failure indicators and development of methods for predicting the remaining useful life of the device in its use conditions (data collection, statistical assessment, prediction models)
- 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) can provide a virtual space (digital mirror) of the system to depict the behavior of the real entity. Normally, the DT is modeled in three dimensions, i.e. the physical entity, virtual model, and connection [12]. A DT-driven PHM includes a five-dimensional architecture with physical model, vertical model, data model, service model and connection model. It makes effective use of the interaction mechanism and fused data of the DT. The development areas that need to be addressed are:

- Predictive reliability modeling and simulation-based optimization
- Multiphysics/multiscale/probabilistic dynamic simulation
- Full lifecycle in-situ monitoring with smart sensors
- Big-data storage with Cloud and processing with deep learning
- Intelligent decision-making with AI
- Intelligent perception and connection technology
- Digital twin data construction and management
- Smart service analysis method based on digital twin data
- Testing strategy and testing platform for verification, i.e. cost-effective testing strategy and test methodologies; automated test pattern generation, data analysis and diagnosis flows; multifunctional performance testing; multi-scale testing; multi domain cross talk; complex system testing
- Smart software
- Cyclic economy management
Digital twin for electronic components and modules (Source: G.Q. Zhang & Jiajie Fan)

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

Table 1. Modeling & Simulation Metrics

<table>
<thead>
<tr>
<th>Metric</th>
<th>5 years</th>
<th>10 years</th>
<th>15 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concept to Product</td>
<td>5 years</td>
<td>3 years</td>
<td>18 months</td>
</tr>
<tr>
<td>Model Accuracy for Reliability</td>
<td>50%</td>
<td>75%</td>
<td>100%</td>
</tr>
<tr>
<td>Products validated through M&amp;S</td>
<td>50%</td>
<td>70%</td>
<td>100%</td>
</tr>
<tr>
<td>AI/Machine Learning</td>
<td>Use of Machine Learning to learn from different designs for single physics</td>
<td>Use of Machine Learning to learn from different designs for multi-physics</td>
<td></td>
</tr>
<tr>
<td>Multi-Physics</td>
<td>Accurate multi-physics analysis for chip-package co-design</td>
<td>Accurate multi-physics analysis for whole system</td>
<td></td>
</tr>
<tr>
<td>Data Sharing</td>
<td>Interfaces between tools and ADK’s and PDK’s</td>
<td>Data and model sharing through supply chain</td>
<td></td>
</tr>
</tbody>
</table>
Table 2: Key developments and achievements required for PoF, DfR and PHM

<table>
<thead>
<tr>
<th>Year</th>
<th>PoF</th>
<th>DfR</th>
<th>PHM</th>
</tr>
</thead>
</table>
| 3    | • Physical failure analysis techniques applicable during the loading situation  
• Realistic material and interface characterisation 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 characterisation  
• Metamodeling and Model Order Reduction: complex behaviour 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 behaviour 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) |

References:
1. EPOSS Reliability Research Challenges, 2017
4. Jedeec standards are available at http://www.jedec.org/
5. W. B. Nelson, Accelerated Testing: Statistical Models, Test Plans, and Data