



HETEROGENEOUS INTEGRATION ROADMAP

2025 Edition

Chapter 14: Modeling & Simulation

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Contents

Executive Summary.....	4
14.1 Use of Modeling and Simulation for Heterogeneous Integrated Systems	6
14.1.1 Physics-Based Models.....	6
Electrical modeling	6
Thermal and mechanical modeling	6
Materials modeling	7
Multi-physics and multi-scale modeling	8
Failure and reliability modeling.....	8
Metrology for modeling and simulation.....	10
Cost and supply-chain models	11
14.1.2 Data-Driven Models.....	11
14.1.3 Digital Twins	12
14.2. State-of-the-Art and Key Attributes for Modeling and Simulation	13
14.2.1 Physics-Based Models.....	13
Electrical modeling	13
Thermal and mechanical modeling	14
Materials modeling	15
Multi-physics and multi-scale modeling	16
Failure and reliability modeling.....	17
Metrology for modeling and simulation.....	18
Cost and supply-chain models	18
14.2.2 Data-Driven Models.....	19
14.2.3 Digital Twins	19
14.3. Future Projections for Modeling and Simulation	21
14.4. Research and Development Directions	23
Metrology-Driven Inputs and Model Validation	23
Process-Model Driven Manufacturing and Yield Optimization	23
Multi-Physics/Scale/Domain Modeling Capability	23
High-Precision Failure Reliability Models	24
AI-Assisted and Fast Simulations to Support Co-Design.....	24
Digital Twin Integration Capability	25
14.5. Key Challenges	25
Metrology-Driven Inputs and Model Validation	25
Process-Model-Driven Manufacturing and Yield Optimization	25
Multi-Physics/Scale/Domain Capability	26
High-Precision Failure Reliability Models	26
AI-Assisted and Fast Simulations to Support Co-Design.....	26

Digital Twin Integration	27
Cross-Cutting Grand Challenges.....	27
Glossary	27
TWG Volunteers.....	28
References.....	28

Figures

Figure 1 Modeling and Simulation for Heterogeneous Integration	5
Figure 2 Predicting the eye diagram for TSMC CoWoS package architecture [2].....	6
Figure 3 Atomistic and molecular dynamics analysis of hybrid bond interface [4]	7
Figure 4 Multi-physics model of wafer warpage due to fan-out wafer packaging process conditions [5]	8
Figure 6 Some examples of failures found in advanced semiconductor packages.....	9
Figure 5 Modeling techniques across the length and time domains	9
Figure 7 80% of the manufacturing cost and performance of a product is committed in the first 20% of the design cycle [8]	11
Figure 8 Digital-twin technologies	13
Figure 9 Digital-twin communication between physical and virtual domains	13
Figure 10 Model order reduction techniques compared to full finite element solver for thermo-mechanical analysis of a power electronics module [12]	15
Figure 11 Multi-physics model for atom migration in interconnects [17]	16
Figure 12 Use of FEA and accelerated life tests to predict damage metrics and failure life model [24]	17
Figure 13 Impact of including grain structure recrystallization in model FEA analysis [25], [26]	18

Tables

Table 1 Some examples of modeling requirements for different failure modes arising from manufacturing process and in-field environmental stress in advanced packaging	10
Table 2 Modeling and simulation projections for near, mid, and long-term	22

Executive Summary

The focus of this chapter is to describe the modeling and simulation capabilities and future requirements for heterogeneous integrated systems. The chapter has the following objectives:

1. Describe different types of modeling and simulation technologies and their application to heterogeneous integration, with a focus on systems.
2. Project in a quantitative and qualitative manner how modeling and simulation technologies and their attributes will evolve in the near, mid, and long term to support the needs of future heterogeneous integration.
3. Detail the research directions that support the projected near-, mid-, and long-term evolution of modeling and simulation advances for heterogeneous integrated chiplet-based systems supported by advanced packaging.
4. Detail the key challenges that must be addressed to realize these projected advances.

As semiconductor systems progress toward 2.5D and 3D heterogeneous integration of electronic components, [1] modeling and simulation capabilities must evolve to address tightly coupled electrical, thermal, and mechanical phenomena across multiple length and time scales, as shown in Figure 1. Device-level effects at the nanometer scale, package-level interactions at micrometer to millimeter-scales, and system-level thermal and mechanical behavior must be treated within a unified multi-physics, multi-scale framework. Existing mesh-based approaches, including finite element and computational fluid dynamics methods, are limited in their ability to span these scales efficiently, particularly when electrical effects occur on nanosecond timescales while thermal and mechanical responses persist from seconds or longer lifetimes.

To close this gap, the roadmap for modeling and simulation requires hierarchical modeling approaches based on abstraction, reduced-order and compact models, efficient sub-modeling and artificial intelligence (AI)/machine learning (ML) techniques. Standardized data exchange between abstraction levels is a key enabler for chip–package–system co-design and co-simulation. As technology nodes advance to FinFET and gate-all-around architectures at 2 nm and below, additional effects such as transistor self-heating and increased chip-package interaction must be taken into account. Long-term progress will depend on integrating physics-based modeling with data-driven methods, supported by improved metrology and in-situ sensing, to establish a robust knowledge base for advanced packaging and heterogeneous integration beyond the limits of traditional Moore’s Law scaling.

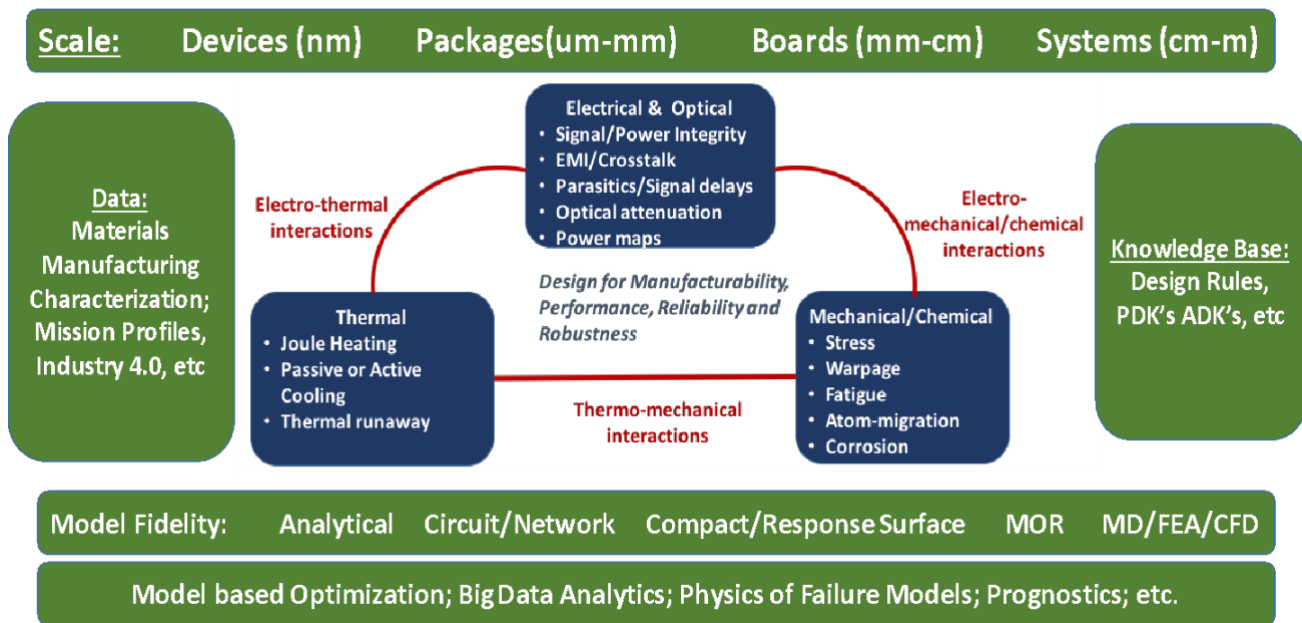


Figure 1 Modeling and Simulation for Heterogeneous Integration

Near-term advances focus on improving the fidelity of physics-based models to accurately capture the electrical, thermal, mechanical, and reliability behavior of increasingly complex packages. These models form the foundation for integrating data-driven techniques, including AI-assisted model calibration and accelerated design-space exploration.

In the mid-term, integrating multi-physics simulation, AI-driven analytics, and in-line metrology will deploy dynamic digital twins that continuously synchronize models with manufacturing and operational data. This precision will empower packaging engineers to validate designs sooner, quantify uncertainty, and address real-world variability across chip, package, and system-level length scales.

Looking toward the long term, modeling and simulation will move from analysis-centric tasks to a closed-loop, autonomous framework for designing and optimizing engineering systems. Digital twins, virtual replicas of physical devices, will evolve to predict product behavior over its entire lifetime, including degradation during everyday use. They will also forecast how different subsystems interact within complex assemblies, enabling proactive reliability management and shorter innovation cycles. Throughout this chapter, tightly linked approaches for modeling at multiple scales (from materials to systems), incorporating different physical phenomena (mechanical, thermal, electrical), and spanning multiple domains (such as cost analysis and supply chain logistics), will be essential. This is especially true as advanced packaging evolves from single-chip solutions to highly integrated, multi-component systems.

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14.1 Use of Modeling and Simulation for Heterogeneous Integrated Systems

14.1.1 Physics-Based Models

Electrical modeling

- Different electrical domains rely on distinct and specialized simulation technologies. For example, digital timing and signal integrity analysis primarily use time-domain and SPICE-based tools. In contrast, high-speed serial links depend on statistical jitter and noise analysis combined with behavioral equalization models. Furthermore, RF and analog/mixed-signal designs are typically evaluated using frequency-domain solvers, while electromagnetic behavior requires full-wave tools that directly solve Maxwell's equations. Despite their importance, these simulation environments operate largely independently, with limited integration or convergence across domains. An example of an electrical modeling calculation is given in Figure 2, where simulations are used to predict eye diagrams [2].

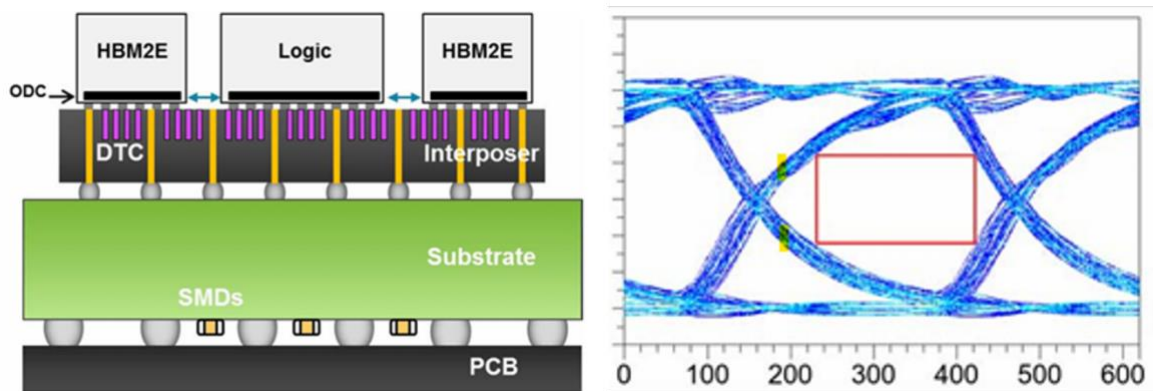


Figure 2 Predicting the eye diagram for TSMC CoWoS package architecture [2]

- At the die level, sub-micron interconnects are electrically much smaller than signal wavelengths, and thus dominant effects include RC delay, signal integrity, and power integrity. As a result, quasi-static field solvers are typically used to extract lumped-element or SPICE models. At the package and PCB levels, interconnect behavior involves a combination of lumped and distributed effects, requiring the use of quasi-static and 3D electromagnetic field solvers for parasitic extraction and the assessment of signal integrity, power integrity, and EMI. As signal speeds and operating frequencies increase, transmission line effects become dominant, necessitating full-wave 3D electromagnetic solvers to compute scattering parameters (S-parameters) for accurate modeling.

Thermal and mechanical modeling

- Thermal modeling is a central modeling and simulation tool in heterogeneous integration and advanced semiconductor packaging. It is used to predict temperatures and hotspots across chiplets, 2.5D/3D stacks, interposers, and complex material systems. It supports early architectural decisions, detailed package optimization, and electro-thermal co-simulation by accounting for temperature-dependent behavior and anisotropic materials. Thermal modeling techniques such as finite-element analysis, thermal-resistance networks, and computational

fluid dynamics, which can be passive and/or active, are used to assess thermal management options in advanced packaging .

- Thermal results are also coupled with mechanical stress analysis to assess stress, warpage, and long-term reliability. In addition, compact and AI-based models enable rapid design-space exploration and runtime thermal management, making thermal analysis a first-order constraint in modern high-power AI and HPC systems. Mechanical modeling is a critical predictive discipline used to ensure the structural integrity and reliability of advanced electronic packaging and system integration. It primarily addresses two fundamental concerns: thermo-mechanical issues and issues arising from external mechanical loads, or a combination of both. Most modeling efforts focus on thermo-mechanical phenomena, where the mismatches in coefficients of thermal expansion among diverse materials, such as silicon, polymers, and metals, induce internal stress, strain, and deformation during thermal cycling.
- These thermal and thermo-mechanical simulations are essential for analyzing fracture, fatigue, and warpage, which often lead to failures like solder joint cracking or thin-film delamination. On the other hand, mechanical modeling also evaluates the impact of physical forces, such as assembly clamping, vibration, and drop impacts. By delivering a quantitative assessment of these stresses through methods like finite element analysis (FEA), mechanical modeling provides the necessary design support to optimize material selection and geometric design. This capability is vital for the successful implementation of high-density interconnects, ultimately ensuring that complex systems remain robust throughout their operational life [3].

Materials modeling

- Materials modeling is increasingly performed through atomistic or molecular modeling methods, such as molecular dynamics (MD) or density functional theory (DFT). As feature sizes shrink and interconnect footprint densities increase, material analysis must undergo a paradigm shift from traditional bulk properties to the study of direct intermolecular or interatomic interactions. Molecular modeling is employed to define the critical differences between bulk and interfacial properties, identifying how specific material interfaces interact and how those interactions transform to initiate failure. By analyzing these systems at the atomistic level, engineers can determine if the risk of using a specific material is warranted, while reliability engineers can pinpoint which material and condition combinations are most vulnerable to degradation. Figure 3 shows an example of atomistic and molecular dynamics analysis [4].

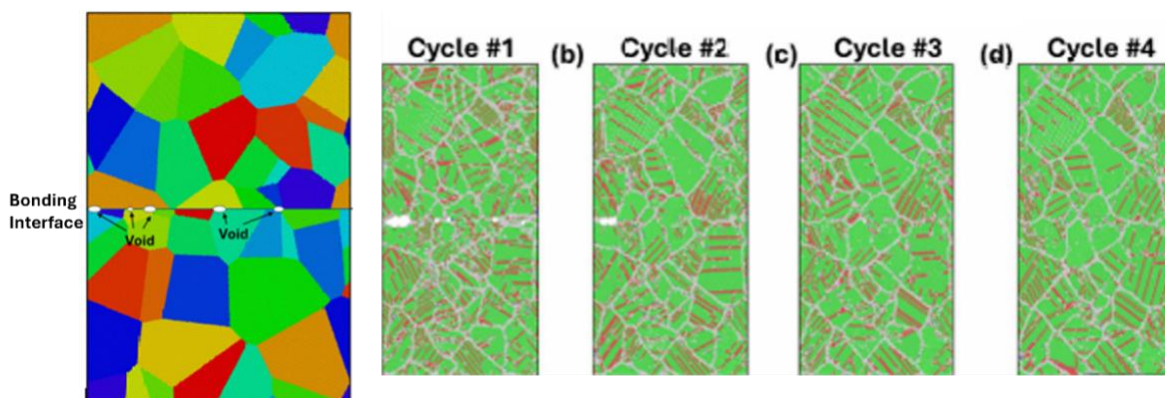


Figure 3 Atomistic and molecular dynamics analysis of hybrid bond interface [4]

- The primary goal of molecular modeling is to predict fundamental thermal, electrical, and mechanical properties of new materials before they are synthesized. This bottom-up approach provides the high-resolution data necessary

to support the design of robust interfaces in next-generation electronic packages, ensuring that atomic-scale behaviors are aligned with macro-scale performance requirements.

Multi-physics and multi-scale modeling

- Heterogeneous integration demands multi-physics and multi-scale modeling to capture the true behavior of complex systems. Electronic packaging often involves coupled interactions across various physical domains, such as electrical, thermal, mechanical, or even humidity, optical, and diffusion factors. For instance, electrical current generates resistive heating, which in turn triggers thermal-mechanical stress, requiring a multi-physics approach to accurately predict performance and reliability. Simultaneously, these systems are multiscale in nature, spanning from the millimeter scale at the system level down to micrometers in interconnect structures and nanometers at the transistor level.
- Manufacturing process models [5]–[7] are inherently multi-physics and multi-scale in nature and scale to capture the behavior of materials from 300mm wafers down to 5 μ m redistribution layers [6]. As detailed in Figure 4, it is important to ensure correct material properties and process conditions are used in the simulation.

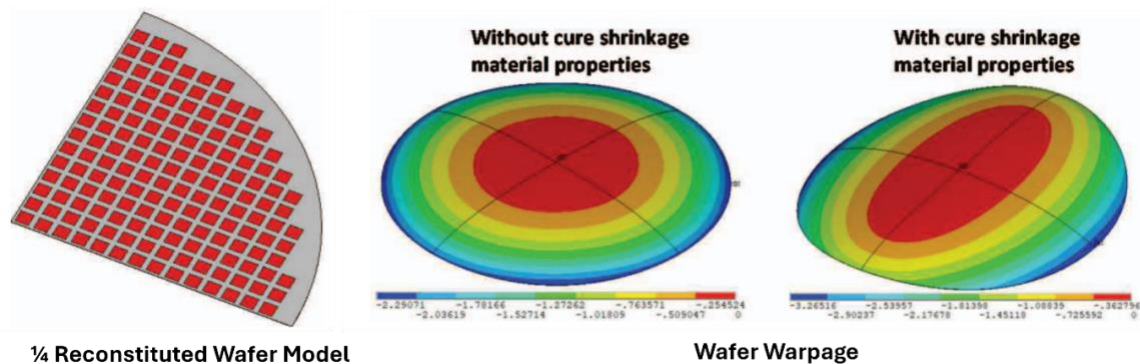


Figure 4 Multi-physics model of wafer warpage due to fan-out wafer packaging process conditions [5]

- Since mechanical failures, such as interfacial delamination or micro-bump cracking, originate at the micro or nano scale, multiscale modeling is essential to bridge these dimensions. By integrating these diverse disciplines and scales into a unified simulation framework, engineers can gain a comprehensive understanding of how nanoscale phenomena influence macro scale system integrity. This holistic modeling approach provides the high-fidelity insights required to optimize high-density architectures, significantly reducing the risk of unforeseen failures in next-generation integrated systems. Figure 5 illustrates the different modeling techniques that can be adopted across the space and time domains.

Failure and reliability modeling

(Further details can be found in Chapter 24.)

- Reliability modeling in electronic packaging is a statistical and physics-based approach used to predict the probability that a system will function over a specified period under defined environmental conditions. While electrical, thermal, mechanical, multi-physics/multi-scale, and materials modeling focus on mechanistic relationships, reliability modeling aims to quantify the long-term durability and life expectancy of the integrated system by integrating experimental data with mathematical distributions, such as the Weibull or Lognormal models, to assess the impact of cumulative damage mechanisms like electromigration, corrosion, thermal fatigue, and others as detailed in Figure 6. Further details on failures and reliability aspects for advanced semiconductor packaging can be found in Chapter 24: Reliability.

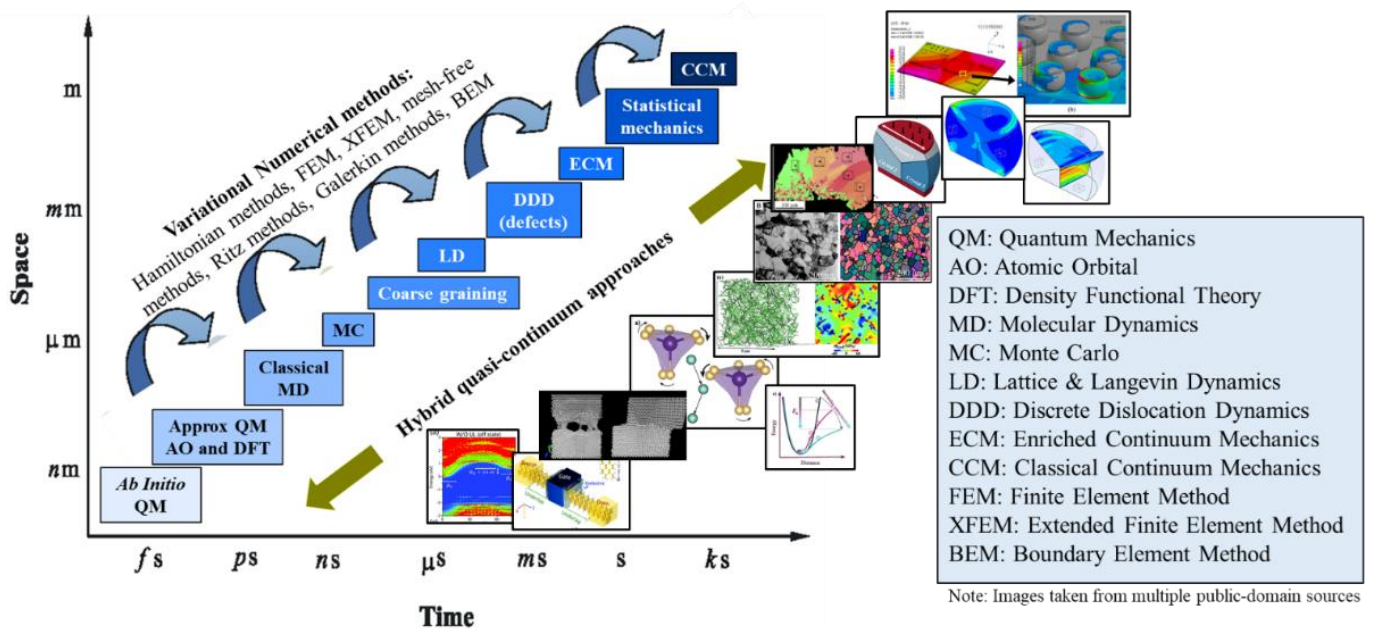


Figure 6 Modeling techniques across the length and time domains

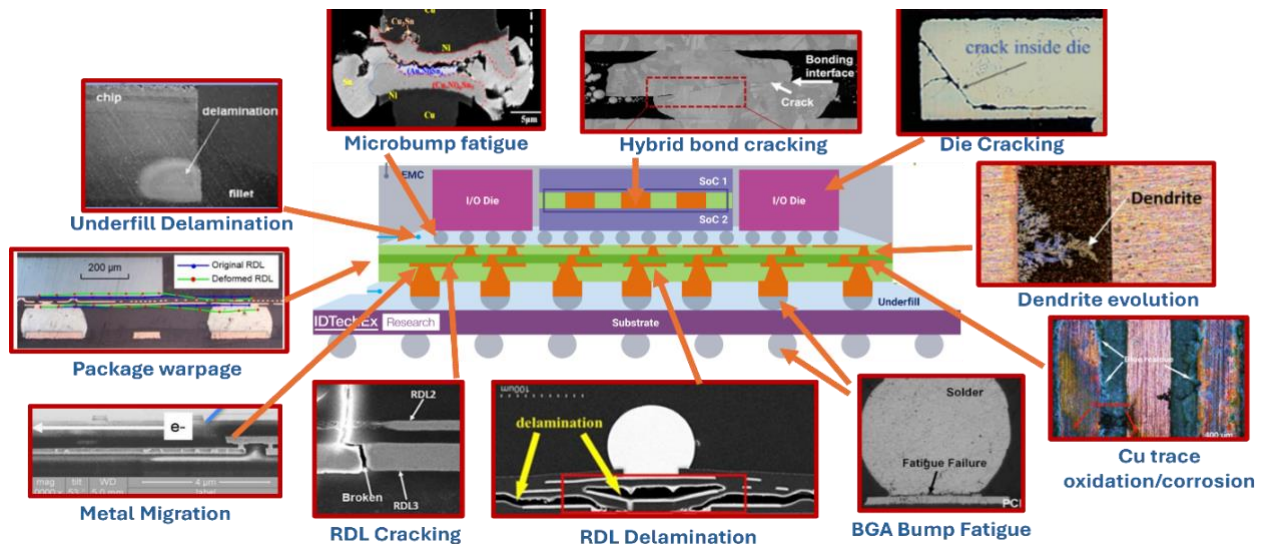


Figure 5 Some examples of failures found in advanced semiconductor packages

- Many of the failures are driven by multi-physics coupled across the die-package-system domains. Reliability modeling for heterogeneous integration has shifted toward physics-informed data science, combining traditional

life-distribution models with real-time health monitoring. Table 1 details the modeling requirements for predicting reliability for different failure modes.

Table 1 Some examples of modeling requirements for different failure modes arising from manufacturing process and in-field environmental stress in advanced packaging

Failure Mode	Modeling requirements
Delamination	- Multi-physics models at system level. Multi-scale modeling. - Coupled micro-mechanical models at local failure sites to predict stress. Adhesion strength at interfaces required
Cracking	- Multi-physics at system level. Multi-scale modeling. - Coupled micro-mechanical models at local failure sites. Fracture toughness.
Wafer and Package Warpage	- Multi-physics models at system level to predict overall warpage during packaging manufacturing processes as wafer warpage impacts assembly yield and reliability. - Multi-physics models also required for package warpage predictions due to in-service loads.
Opens/Shorts	Multi-physics manufacturing process models (plating, etching, etc). For example, predicting RDL metal shorts due to over-etch, bridging or opens (cracks, voids, under-etch)
Die Shift/Misalignment	Die shift during molding causes interconnect misalignment. Addressed by adaptive patterning.
Metal Migration	- Multi-physics models at system level. Multi-scale modeling. - Coupled micro-mechanical models at local failure sites to predict stress.
Oxidation/Corrosion	- Multi-physics models at system level. Multi-scale modeling. - Coupled micro-mechanical models at local failure sites to predict stress.

- By delivering predictive failure rates (the probability that a system or component will fail during a specific period) and mean time to failure metrics (the average operating time between inherent failures), reliability modeling provides the ultimate results for risk assessment, ensuring that complex systems meet the stringent longevity requirements of industries such as automotive, aerospace, and high-performance computing.

Metrology for modeling and simulation

- Metrology is essential for accurate modeling and simulation in heterogeneous integration and advanced packaging. It aims to provide accurate, high-resolution measurements of material properties, constitutive responses, geometries, and defects. It ensures that simulation inputs reflect real-world behavior, including process-dependent effects, temperature and moisture-dependent effects, and evolving behavior due to aging and damage accumulation across polymers, metals, and interconnects.
- Through model calibration and validation, metrology enables highly accurate predictions of reliability, yield, and performance. Additionally, it supports the identification of failure modes and types of damage progression, as well as providing essential data for development of failure criteria such as crack growth laws and fatigue criteria. Ultimately, metrology-driven modeling will allow the creation of reliable digital twins and simulation tools that can guide design, process optimization, manufacturing decisions, and overall product reliability.

Cost and supply-chain models

- Cost and supply-chain models for heterogeneous integration and advanced packaging aim to provide data-driven guidance across design, manufacturing, and logistics. These models seek to enable accurate prediction and optimization of manufacturing cost by evaluating trade-offs between yield, reliability, materials, and process complexity. Figure 7 details the importance of applying cost modeling together with performance modeling.

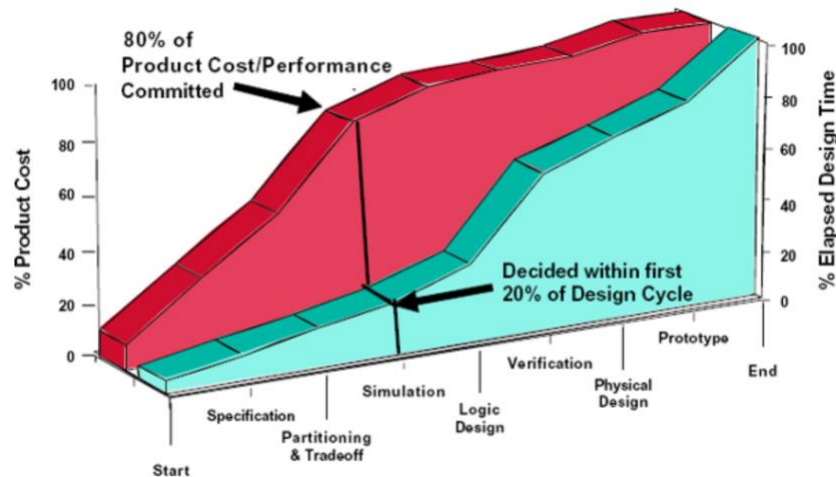


Figure 7 80% of the manufacturing cost and performance of a product is committed in the first 20% of the design cycle [8]

- These cost models, together with performance models, help maximize product quality and yield through predictive analysis of defects, process variations, and assembly tolerances, as well as minimize associated costs. They also aim to support supply chain resilience and scalability by simulating global networks, capacity constraints, lead times, and risks.
- By integrating data from metrology, production, and logistics, these models inform critical decisions on material selection, process choices, and packaging architectures, ensuring optimal performance, cost efficiency, and time-to-market.

14.1.2 Data-Driven Models

- Data-driven models are emerging as a critical complement to physics-based modeling and simulation for heterogeneous integration (HI), driven by increasing system complexity, expanding design spaces, and the prohibitive computational cost of exhaustive multi-physics simulations. Rather than replacing physics-based approaches, data-driven models leverage simulation, experimental, and in-field data to enable faster prediction, design space exploration, and optimization across chip–package–board–system domains.
- In the context of HI, data-driven modeling primarily addresses challenges associated with scale, speed, and uncertainty. As heterogeneous systems integrate diverse functions (digital, RF, power, photonics, sensing) and span multiple length and time scales, conventional simulation workflows struggle to support early-stage co-design and iterative optimization. Data-driven approaches enable surrogate representations of complex physical behavior that can be evaluated orders of magnitude faster than full-fidelity models, making them suitable for system-level trade studies and design closure. Today, data-driven models are used to produce reduced-order models (ROMs) that are being further advanced using ML and AI techniques.

- Reduced-order models are a foundational class of data-driven techniques. ROMs distill high-fidelity simulation results or measurement data into compact representations that preserve dominant system behavior while dramatically reducing computational cost. In HI applications, ROMs support rapid evaluation of electrical, thermal, and mechanical responses at the package and system levels, enabling early feedback between domains and facilitating co-simulation workflows that would otherwise be impractical.
- Machine learning (ML) and artificial intelligence (AI) techniques extend data-driven modeling. They capture nonlinear interactions, high-dimensional dependencies, and statistical variability in heterogeneous systems. ML-based models can be trained on simulation outputs, manufacturing, or operational data. These models predict metrics such as signal integrity margins, thermal hot-spot evolution, power integrity behavior, or reliability indicators. These techniques are valuable for uncertainty quantification, sensitivity analysis, and identification of critical design parameters in large design spaces.

14.1.3 Digital Twins

- Digital twins and technology co-optimization represent a system-level evolution of modeling and simulation, integrating physics-based and data-driven models with real-time data into a unified framework spanning design, manufacturing, and operations, as shown in Figure 8 and Figure 9. For heterogeneous integration, digital twins provide a mechanism to manage complexity across the full lifecycle of advanced electronic systems.
- A digital twin in the HI context is a dynamic, continuously updated virtual representation of a component, package, or system that reflects its physical state through linkage with simulation models, metrology measurements, and embedded sensing. Unlike static models used during design, digital twins evolve over time, incorporate process variations, environmental conditions, aging, and operational stress, and damage accumulation. This enables prediction of system behavior beyond nominal conditions and supports in-field monitoring, diagnostics, and prognostics.
- Technology co-optimization uses digital twins to connect decisions across silos like device technology, packaging, thermal management, power delivery, and system integration. In HI, chiplet-based architectures and advanced packaging mean no single design layer defines performance. Digital twins help designers see trade-offs clearly and balance electrical, thermal, mechanical, reliability, and cost needs.

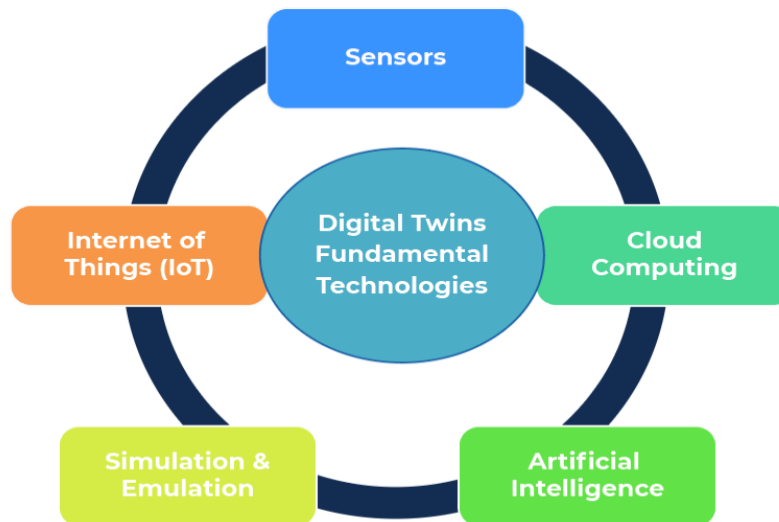


Figure 8 Digital-twin technologies

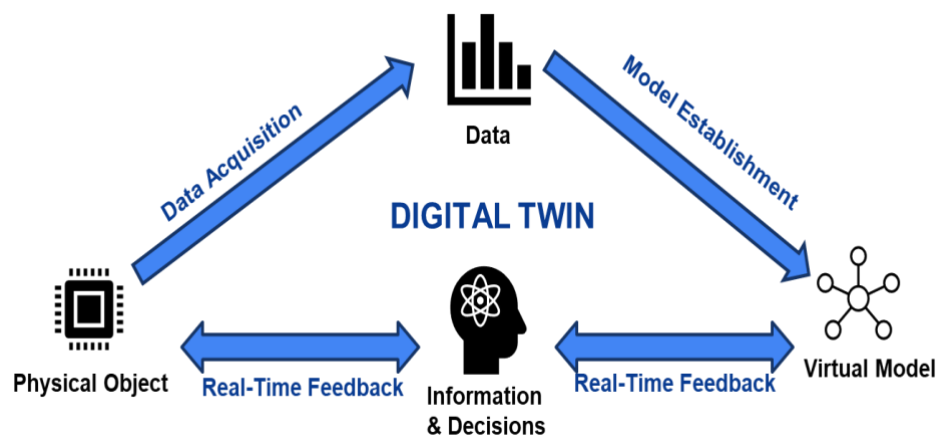


Figure 9 Digital-twin communication between physical and virtual domains

14.2. State-of-the-Art and Key Attributes for Modeling and Simulation

14.2.1 Physics-Based Models

Electrical modeling

- State-of-the-art techniques combine electromagnetic (EM) field solvers, equivalent circuit modeling, and multi-physics simulations to achieve high-fidelity representations of package behavior across wide frequency ranges. Three-dimensional full-wave solvers are widely used to extract parasitic parameters and S-parameters, particularly for RF and millimeter-wave applications. For power electronics, partial element equivalent circuit (PEEC) methods and reduced-order models are commonly employed to balance accuracy and computational efficiency.
- Advanced packaging technologies—such as flip-chip, wafer-level packaging (WLP), 2.5D/3D integration, and system-in-package (SiP)—require increasingly detailed models that account for complex geometries,

heterogeneous integration, and strong electromagnetic coupling effects. Co-design methodologies that integrate chip, package, and PCB modeling have become essential to ensure signal integrity (SI), power integrity (PI), and electromagnetic compatibility (EMC).

- Recent developments also include model order reduction (MOR) techniques, broadband macromodel generation, and machine learning-assisted parameter extraction to accelerate simulation workflows while maintaining accuracy. Thermal-electrical coupling is frequently incorporated to account for temperature-dependent material properties and self-heating effects.
- Additionally, improvements in domain decomposition methods (DDMs) for combining different types of electronic components—such as those found in 2.5D/3D integrated circuits—have enabled the division of large, complex systems composed of different materials into smaller, more manageable parts. This speeds up the simulation and enables parallel execution of tasks. DDMs tackle complicated shapes and mismatched materials by solving each part separately. The main types of domain decomposition methods are: Domain decomposition and reduction (DDR), which breaks down and simplifies problems; non-overlapping methods, such as Schur Complement and FETI, which solve separate parts and coordinate at the edges; and overlapping methods, like the Schwarz algorithm, where parts share some regions and update solutions together. These methods make computations more efficient, require less memory, and speed up simulations of large, mixed systems. They also help by allowing different computers to work on separate parts simultaneously and by connecting subsystems, which is useful for linking different physical effects or materials in 2.5D/3D electronics [9], [10].
- Building on these developments, the current state of the art emphasizes key attributes such as high accuracy, broadband capability, multi-physics integration, and computational efficiency to support next-generation semiconductor devices operating at increasingly demanding performance levels.

Thermal and mechanical modeling

- State-of-the-art thermal modeling for heterogeneous integration and advanced semiconductor packaging combines detailed 3D finite-element/finite-difference/or finite-volume simulations with compact and reduced-order models to balance accuracy and computational efficiency. These methods aim to capture complex geometries (chipllets, TSVs, microbumps, interposers), anisotropic and temperature-dependent materials, and strong hotspot behavior in 2.5D/3D stacks. Increasingly, electro-thermal and thermo-mechanical coupling is being integrated into chip–package co-design flows to assess performance and reliability early in development. In parallel, AI-based surrogate and data-driven models are being adopted to accelerate design space exploration and enable system-level optimization for high-power AI and HPC systems.
- At the die level, circuit performance and power become increasingly sensitive to thermal and mechanical effects from chip and packaging level. Multi-physics co-design techniques are being developed to optimize timing and voltage drop in early design stage and accelerate time to sign-off.
- State-of-the-art thermal modeling for heterogeneous integration and advanced semiconductor packaging combines detailed 3D simulations with compact and reduced-order models [11]. This balances accuracy and computational efficiency. These methods capture complex geometries (chipllets, TSVs, microbumps, interposers), anisotropic and temperature-dependent materials, and strong hotspot behavior in 2.5D/3D stacks. Electro-thermal and thermo-mechanical coupling now enhances chip–package co-design flows, enabling early assessment of performance and reliability. In parallel, AI-based surrogates and data-driven models accelerate design-space exploration and enable system-level optimization for high-power AI and HPC systems.
- The state of the art in mechanical modeling is evidenced by the wide adoption of finite element analysis (FEA), which has proven highly successful in predicting solder joint fatigue, interface delamination, thin film cracking, and

failures related to drop, impact, or vibration. Model order reduction (MOR) techniques also provide benefits in terms of significantly reducing compute time compared to a full finite element analysis as detailed in Figure 10, where MoR techniques provide > 80% reduction in computational speed without loss of accuracy when compared with a full finite element model [12].

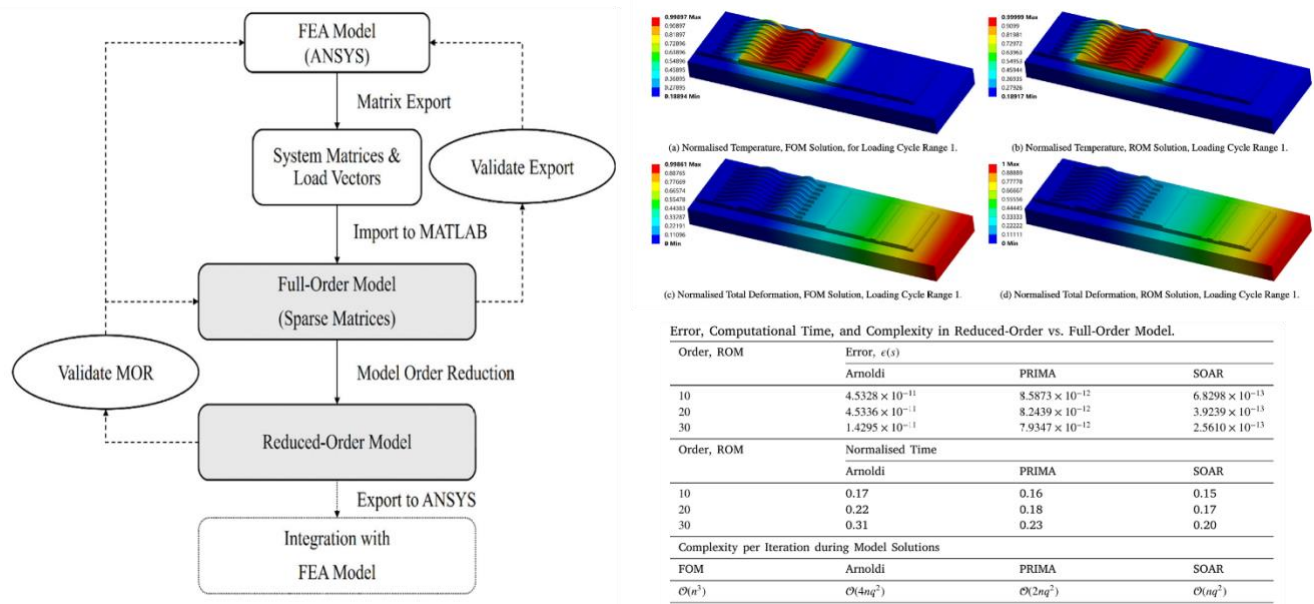


Figure 10 Model order reduction techniques compared to full finite element solver for thermo-mechanical analysis of a power electronics module [12]

- Advanced constitutive models are being developed for solder and polymer-based encapsulant materials that have evolving properties due to aging effects, moisture adsorption, and damage accumulation. In addition, constitutive models and material properties are needed for new materials that are continually being developed to address performance enhancement goals. These model developments are supported by advanced material characterization methods and metrologies to accurately determine responses and properties.
- Machine learning is emerging as a powerful tool to accelerate modeling processes without a loss of accuracy.
- Key attributes for thermal-mechanical modeling must include accurate capture of complex 3D structures and material behavior while remaining computationally efficient and scalable. Models should support transient and multi-physics analysis, integrate into design workflows, and enable reliable prediction of hotspots and long-term performance. In addition, models should include mesh automation for complex systems, be supported by precise material characterization, and enable the determination of key metrics to define and support robust failure criteria for complex integrated systems.

Materials modeling

- Materials modeling in heterogeneous integration is increasingly used to predict fundamental properties, such as interfacial adhesion, thermal conductivity, moisture diffusivity, and complex thermal mechanical behaviors using molecular dynamics (MD), density functional theory (DFT), and crystal plasticity approaches [13]–[16].

- Atomistic modeling has become a cornerstone for developing new materials tailored for high-density interconnects and advanced new materials. Furthermore, atomistic simulations provide correlations between macro-scale failure mechanisms with findings of atomistic evolution, providing a deeper understanding of failure mechanisms. Finally, crystal plasticity simulations can be used to establish the complex constitutive behaviors of small interconnections and thin layers that contain only a small number of anisotropic grains that include multiple slip systems.
- Key attributes of this field include the introduction of machine-learned interatomic potentials, which allow for thermal, mechanical, and structural simulations of a wider range of novel materials. This pushes the boundary on the complexity of systems to which atomistic modeling can accurately and efficiently be applied, thus establishing a more robust connection between atomistic-level and continuum modeling to inform system-level design.

Multi-physics and multi-scale modeling

- Multi-physics and multi-scale modeling have been rapidly evolving in recent years and are characterized by the integration of software platforms, such as Synopsis/ANSYS, Cadence, and COMSOL, which provide capabilities for electro-thermal-mechanical co-simulation and coupled thermal-moisture-mechanical modeling. In addition, as illustrated in Figure 11, significant advancements have been made in developing new mathematical formulations for electromigration, coupling electrical, thermal, diffusion, and mechanical fields and verifying them experimentally.

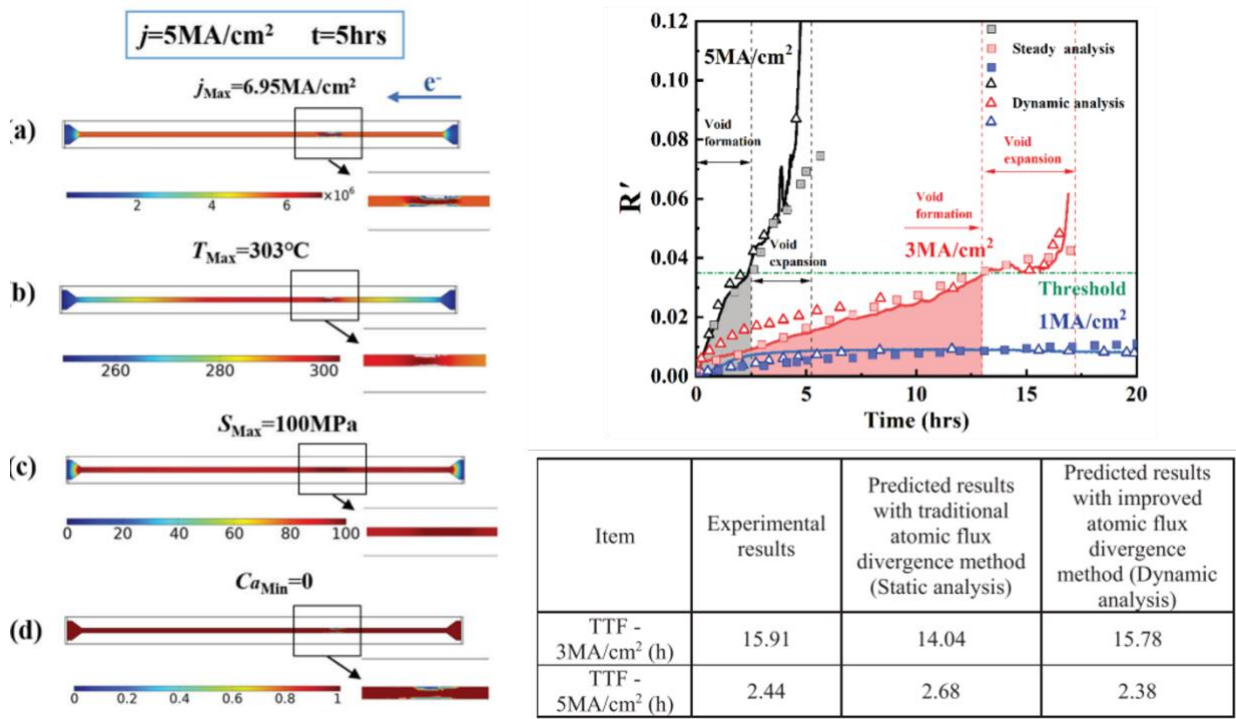


Figure 11 Multi-physics model for atom migration in interconnects [17]

- The state-of-the-art capabilities for multi-physics and multi-scale modeling have been demonstrated to enable heterogeneous integration of a 2nm SOC with HBM on an RDL interposer, and to balance the interplay of thermal, power, timing, and stress effects in a 3DIC system.
- Multi-scale modeling has become vital for interface integrity prediction, utilizing a hierarchy of methods from molecular dynamics to coarse-grain techniques and cohesive zone finite element analysis.

- Key attributes of this field include the development of coupled constitutive models, the bridging of multiple length-scales and multiple time-scales for modeling from atomistic level to continuum level, the ability to capture evolution of material properties with progressive aging throughout the life-cycle, and the continuous improvement of computational efficiency to manage the time-consuming, complex, coupled simulations [17]–[23].

Failure and reliability modeling

(Further details can be found in Chapter 24.)

- Reliability modeling for heterogeneous integration has shifted toward physics-informed data science, combining traditional life-distribution models with real-time health monitoring. As complexity rises in 3D-stacked architectures, the industry is moving toward digital twin technology, where virtual replicas of packages are updated with in-situ sensor data to provide dynamic reliability assessments.
- Current modeling techniques use a combination of data from accelerated life tests and finite element predictions. When FEA results, such as creep strain energy accumulation in solder bumps, are used in damage metrics in life models such as the Coffin-Manson and Morrow models, correlation between model and test data provides the parameters for the life models as illustrated in Figure 12 [24].

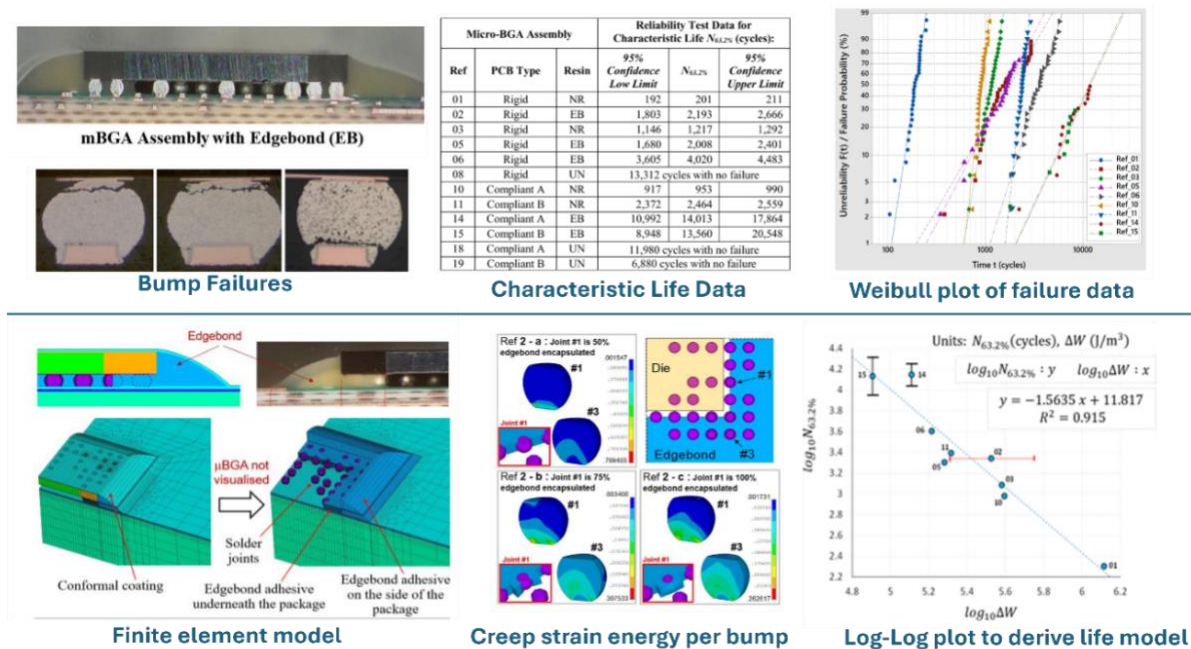


Figure 12 Use of FEA and accelerated life tests to predict damage metrics and failure life model [24]

- As interconnects become smaller, the impact of microstructure cannot be ignored. Several models are now incorporating the changes in microstructure at the micro-level using RVE's. Figure 13 details an example, where the recrystallization is seen to increase the local creep deformation and failure risks, compared to a homogeneous model prediction [25], [26].

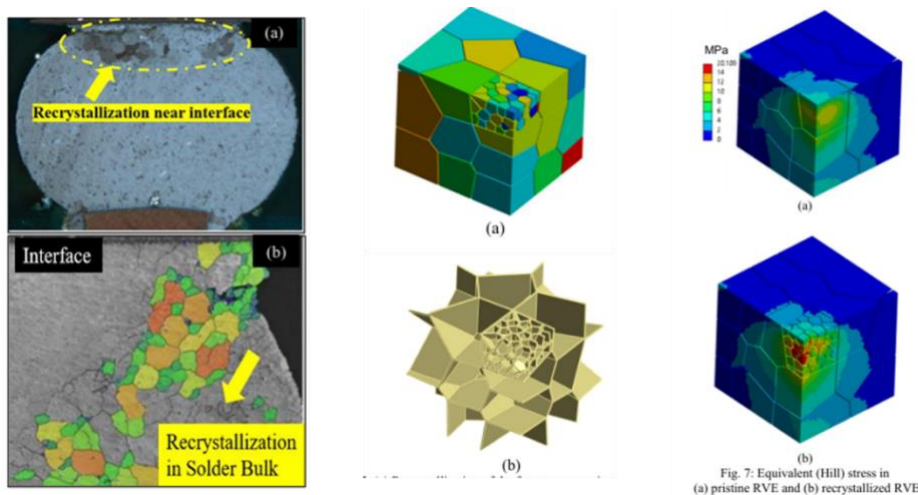


Figure 13 Impact of including grain structure recrystallization in model FEA analysis [25], [26]

- Building on these advancements, current methodologies leverage machine learning algorithms to predict the remaining useful life of interconnects by analyzing multi-dimensional data from accelerated life tests.
- Standards such as IPC/JEDEC-9301 [27] are needed to guide packaging engineers in the use of modeling and simulation techniques for package design and reliability.
- Key attributes of reliability modeling include a reliable experimental database, sophisticated algorithms, and accurate extrapolations to the operational lifetime domain.

Metrology for modeling and simulation

- Current metrology techniques for advanced semiconductor packaging enable high-resolution characterization of materials, geometries, and microstructures critical for accurate modeling and simulation.
- Techniques such as nano-indentation, scanning electron microscopy (SEM), focused ion beam (FIB) cross-sectioning, X-ray tomography, and atomic force microscopy (AFM) provide localized measurements of mechanical, thermal, and electrical properties. These methods allow quantification of process-dependent and miniaturized effects in polymers, metals, and interconnects, supporting calibration and validation of predictive models.
- Verification testing and the derivation of failure modes and criteria are also crucial for simulation accuracy, which is a fundamental requirement for tools like digital twins. However, knowledge of damage accumulation, crack growth, and fatigue failure in electronic interconnects remains limited, and existing analytical models can significantly overestimate the fatigue life of solder joints subjected to mission-profile loads.
- While metrology has advanced significantly, challenges remain in capturing long-term degradation, fatigue, and reliability behavior at the scale required for digital twins and then integrating these measurements into multi-physics and multi-scale simulation frameworks.

Cost and supply-chain models

- Current cost and supply-chain models for heterogeneous integration combine physics-based simulation, yield analysis, and partial digital twins. They use historical and metrology data to predict cost, yield, and reliability, and

can model supply-chain constraints and risks. However, these tools are often siloed, lack full integration across design, manufacturing, and logistics, and real-time, end-to-end optimization remains a key research challenge.

14.2.2 Data-Driven Models

- Data-driven models within heterogeneous integration (HI) are characterized less by specific physical solvers and more by their ability to extract, generalize, and deploy knowledge across large and complex design spaces. In the current state of the art, these models are primarily used to augment physics-based simulation by improving speed, scalability, and uncertainty management across chip–package–board–system domains [28]–[33].
- A key attribute of data-driven models is computational efficiency relative to fidelity. Reduced-order models (ROMs) and surrogate models are evaluated based on how accurately they reproduce relevant system-level metrics (e.g., temperature, stress, signal integrity margins, power integrity response) while achieving orders-of-magnitude reduction in runtime compared to full-fidelity multi-physics simulations. Today, this trade-off is often assessed qualitatively; future HI workflows require standardized quantitative measures of accuracy versus speed.
- Another critical attribute is training data provenance and quality of the training data. Specifically, current data-driven models are typically trained using a combination of simulation outputs, targeted experiments, and limited manufacturing or test data. The relevance of a data-driven model to HI depends strongly on whether training data adequately spans process variation, environmental conditions, and operating modes. Therefore, attributes such as data coverage, representativeness, and traceability to physics-based models or measurements are increasingly important.
- Generalization and robustness are additional distinguishing attributes. Many current machine-learning and AI-assisted models perform well only within narrowly defined design spaces. For HI applications, models must maintain predictive capability when extrapolating across packaging technologies, materials, or integration schemes. Metrics related to uncertainty quantification, confidence bounds, and sensitivity to unseen conditions are therefore essential.
- Interoperability with existing design flows is also a defining attribute. Data-driven models must integrate with electronic design automation (EDA), mechanical CAD (MCAD), and system-level tools to support co-design. Today, this integration is largely ad hoc; standardized interfaces, data formats, and validation metrics are required to enable broader adoption across the HI ecosystem.

14.2.3 Digital Twins

- Digital twins and technology co-optimization extend modeling and simulation beyond design-time analysis into lifecycle-aware, system-level decision frameworks. In the current state of the art, digital twins are emerging as loosely coupled combinations of simulation models, metrology, and operational data rather than fully integrated, continuously synchronized system representations [34]–[36].
- A primary attribute of a digital twin is the degree of coupling between models and physical data. Today, most implementations rely on offline calibration using measurement data. For HI, future digital twins must support near-real-time updates using in-situ sensors, process monitors, and field data. Attributes such as update latency, synchronization fidelity, and data assimilation capability are therefore critical.
- Another key attribute is multi-domain coverage. Effective digital twins for heterogeneous systems must span electrical, thermal, mechanical, and reliability domains across chip, package, and system levels. Currently digital

twins often focus on a single domain or hierarchy level; progress toward HI-relevant digital twins requires measurable capability to represent cross-domain interactions and their impact on system performance.

- For technology co-optimization, an essential attribute is visibility into trade-space across integration layers. Co-optimization frameworks are assessed by their ability to evaluate trade-offs among device technology, packaging architecture, power delivery, thermal management, reliability, and cost. Today, these trade-offs are often evaluated sequentially or qualitatively; quantitative, system-level metrics are needed to compare alternative integration strategies.
- Lifecycle continuity is a further defining attribute. Digital twins and co-optimization frameworks should support transitions from design to manufacturing to operation and back to next-generation design. Attributes related to model reuse, version control, and feedback incorporation from manufacturing and field operations are currently immature but central to long-term HI objectives.
- Data security and IP protection are increasingly important attributes. As digital twins rely on shared models and data across organizational boundaries, mechanisms (such as encryption) for secure data exchange, abstraction, and access control are required to enable adoption without compromising proprietary information.

14.3. Future Projections for Modeling and Simulation

As discussed above, each modeling and simulation tool and its applications have specific attributes that detail their performance and capability. Table 2 lists six key attributes pertaining to modeling and simulation, along with projections related to their development.

- **Near-term advances** focus on improving the fidelity of physics-based models. These models must accurately capture the electrical, thermal, mechanical, and reliability behavior of increasingly complex packages. These models form the foundation for integrating data-driven techniques, such as AI-assisted model calibration and accelerated design-space exploration.
- **In the mid-term**, the convergence of multi-physics simulation, AI-driven analytics, and in-line metrology will enable the deployment of dynamic digital twins that continuously align models with manufacturing and operational data. This capability will allow packaging engineers to validate designs earlier, quantify uncertainty, and account for real-world variability across chip, package, and system-level length scales.
- **Looking to the long term**, modeling and simulation will transition from an analysis-centric function to a closed-loop, autonomous design and optimization framework. Digital twins will evolve to predict lifetime behavior, in-field degradation, and system-level interactions for heterogeneous assemblies, enabling proactive reliability management and faster innovation cycles. Across this roadmap, tightly coupled multi-scale, multi-physics modeling will be essential as advanced packaging scales from single-chip solutions to highly integrated, heterogeneous systems.

Table 2 Modeling and simulation projections for near, mid, and long-term

Future projections for modeling and simulation to support HI requirements			
Key attribute	Near-term	Mid-term	Long-term
Metrology-driven inputs and model validation	• Inline warpage, alignment, and thermal data calibrate models. • Simulation-to-package correlation becomes routine. • Thermal measurement (IR, micro-sensors) used to refine 3D stack models	• Automated model updating based on in-line inspection data. • 3D tomography integrated with stress and defect simulations. • Statistical calibration of variability models.	• Continuous model updating from fab and field data. • Cross-layer defect propagation modeling.
Process-model driven manufacturing and yield optimization	• Chiplet partitioning includes yield modeling at architecture stage. • Monte Carlo variability in RDL, TSV, hybrid bonding.	• Full-stack yield modeling (die + package + substrate). • Architecture-level yield optimization across chiplets.	• Real-time yield-driven architecture synthesis. • Near-zero physical iteration cycles.
Multi-Physics/Scale/Domain modeling capability	• Standard chip–package–board co-simulation. • Transient electro-thermal-mechanical modeling for high-power AI devices.	• Unified concurrent solvers (electrical-thermal-mechanical-chemical). • Power integrity dynamically linked to temperature fields.	• Fully coupled electro-thermo-mechanical-fluid simulation. • Real-time system physics modeling.
High-precision failure reliability models (further details can be found in Chapter 24)	• Embedded electromigration, fatigue, delamination models in design flows. • Evolving properties included in simulations. • Virtual qualification before fabrication	• Coupled multi-physics lifetime prediction. • Failure models reflect evolving material behavior.	• Self-learning reliability engines. • In-field failure prediction and mitigation.
AI-assisted and fast simulations to support Co-Design	• Surrogate models reduce runtime 10–50×. • Package-level digital twins for validation. • Reduced physical prototyping cycles.	• Generative 3D stack exploration. • Multi-objective optimization (power, cost, yield).	• Autonomous heterogeneous system generation. • Millions of design options evaluated in real time.
Digital twin integration capability	• Package-level digital twins for validation. • Reduced physical prototyping cycles.	• Manufacturing-connected twins. • Predictive reliability during production ramp.	• End-to-end digital twin (design → packaging fab → field). • Closed-loop optimization across product generations.

14.4. Research and Development Directions

Metrology-Driven Inputs and Model Validation

- Research and development in metrology-driven modeling must aim to tightly integrate physical measurement with simulation throughout the entire lifecycle of heterogeneous integration. In the near term, this requires advancing high-resolution 3D characterization techniques capable of resolving hybrid bonding interfaces, micro-bump geometry and grain orientation variations, and wafer- or panel-level warpage with high spatial fidelity.
- Mid-term R&D should focus on statistical model calibration using high-volume manufacturing data, including AI-driven detection should target process drift and anomaly signatures that influence reliability and yield.
- Long-term development should support autonomous model updating in which packaging metrology and in-field sensor data continuously refine simulation parameters, enabling predictive adjustments to design rules and process windows. The ultimate objective is a closed-loop validation ecosystem where models are continuously synchronized with physical behavior, eliminating static correlation cycles.

Process-Model Driven Manufacturing and Yield Optimization

- Near-term work should emphasize stochastic modeling of hybrid bonding defects, TSV void formation, RDL linewidth variability, and panel-level warpage, supported by Monte Carlo simulations to quantify sensitivity and process window margins. Physics-based modeling of molding, curing shrinkage, electroplating uniformity, and reflow-induced stress should be incorporated into design-for-manufacturability workflows. Effective multi-physics and multi-scale modeling techniques for key heterogeneous integration technologies such as wafer-scale modeling of CMP and hybrid bonding are highly desirable.
- Mid-term research should deliver full-stack yield modeling frameworks that relate interconnect-level variability to reliability and substrate-induced stress, allowing chiplet partitioning strategies to account for compound yield effects. AI-driven defect clustering and root-cause analytics should feed back into design optimization engines, enabling dynamic tradeoffs among performance, cost, and manufacturability.
- Over the long term, R&D should enable real-time yield-aware architecture synthesis informed by live fab conditions, incorporating stochastic material-level defect propagation and adaptive routing strategies.

Multi-Physics/Scale/Domain Modeling Capability

- Near-term priorities include robust chip–package–board co-simulation environments capable of handling high-speed die-to-die interfaces and power delivery networks under transient workloads, alongside transient electro-thermal modeling for AI and HPC packages with power densities exceeding 1kW. Reduced-order modeling techniques are essential to accelerate large-system simulation without sacrificing fidelity.
- Mid-term research should develop fully concurrent electro-thermo-mechanical solvers that replace loosely coupled sequential approaches, integrating temperature-dependent material properties, stress-induced resistivity changes, and advanced cooling mechanisms such as embedded microfluidics. Hierarchical multi-scale modeling—from nanoscale hotspot generation to board-level heat spreading—must allow abstraction switching while maintaining physics consistency.

- Long-term development should integrate additional domains such as fluid dynamics, chemical diffusion, photonics, and RF behavior into unified simulation frameworks capable of real-time system-level analysis during workload execution. The ultimate goal is seamless, continuously coupled multi-physics/scale modeling that supports architecture co-design rather than post-design validation.
- Research in cost and supply chain modeling for heterogeneous integration and advanced packaging should focus on developing integrated cost-performance frameworks that capture trade-offs among yield, reliability, and manufacturing complexity. Predictive yield and defect analysis using metrology and historical data, along with digital twins of global supply chains, can improve resilience and scalability. Additional directions include real-time supply chain monitoring, multi-objective optimization of cost, performance, and time-to-market, and AI-driven predictive modeling to accelerate simulations and support data-driven decision-making across complex packaging ecosystems

High-Precision Failure Reliability Models

(Further details can be found in Chapter 24.)

- Near-term efforts should refine physics-of-failure models for electromigration, thermo-mechanical fatigue, dielectric breakdown, and interfacial delamination in ultra-fine-pitch and hybrid-bonded structures. Crack initiation and propagation models must incorporate microstructural material behavior and thermal cycling effects. Additional focus should be placed on ingress-related effects (due to moisture, dust, etc.) on reliability.
- Mid-term research should couple these mechanisms into integrated lifetime prediction engines that simultaneously account for current density, stress evolution, and temperature gradients across stacked systems. Physics-informed AI models trained on the fusion of physics-based models with accelerated stress test data and field returns can augment deterministic models, enabling earlier and more accurate forecasting.
- Mid- and Long-term research should consider the scalability of modeling strategies needed to address advanced failure mechanisms (fracture, fatigue, and others). Currently supported methods (for example, the explicit modeling of traces, vias, and other structures) provide a high-degree of accuracy but are still computationally expensive.
- Long-term development should yield self-learning reliability frameworks (exploiting physics-informed neural networks (PINNS), for example) that ingest fleet-level operational data to continuously update degradation parameters and predict failure risk in real time.

AI-Assisted and Fast Simulations to Support Co-Design

- Near-term work should focus on surrogate modeling techniques that replicate high-fidelity finite element and electromagnetic results at a fraction of computational cost, enabling rapid evaluation of warpage, stress, and thermal hotspots. Multi-objective optimization engines should integrate constraints spanning signal/power integrity, yield, cost, and reliability. Adaptive abstraction methods must allow dynamic switching between reduced-order and detailed physics models during co-design workflows.
- Mid-term research should enable generative design systems capable of proposing 3D stack topologies, TSV placements, RDL routing strategies, and cooling architectures based on defined performance objectives. AI systems should manage large-scale distributed simulations across cloud-native high-performance computing infrastructures.

- Long-term directions envision autonomous heterogeneous integration platforms capable of evaluating millions of design permutations in near real time, with engineers providing constraints, governance, and validation rather than manual iteration. This progression redefines simulation from an analysis tool into a generative design engine.

Digital Twin Integration Capability

- Near-term development should focus on package-level digital twins used for virtual qualification, ramp simulation, and sensitivity analysis, integrating selected fab metrology inputs.
- Mid-term research should create manufacturing-connected twins that automatically update simulation parameters based on inline inspection data, enabling predictive ramp optimization and early detection of systemic reliability risks. Reliability digital twins should track degradation trajectories across product lifetimes, correlating workload conditions with stress accumulation.
- Long-term development should enable full end-to-end digital ecosystems spanning design, fabrication, deployment, maintenance, and recycling, incorporating fleet-level analytics and predictive maintenance capabilities. In this mature state, digital twins act as operational intelligence platforms, enabling closed-loop optimization across product generations and transforming heterogeneous integration into a continuously learning system architecture paradigm.

14.5. Key Challenges

Metrology-Driven Inputs and Model Validation

- It is difficult to achieve measurement resolution and accuracy at sub-micron and sub-100 nm scales without destructive analysis (such as for hybrid bonding interfaces and ultra-fine pitch interconnects). Many critical defects (mis-aligned voids, micro-cracks, interface contamination) are buried and are not easy to detect in-line.
- Data integration presents a significant challenge—metrology tools generate massive, heterogeneous datasets (optical, X-ray, acoustic, thermal) that are not naturally structured for direct use in simulation. Converting raw inspection data into calibrated model parameters requires robust feature extraction and uncertainty quantification. Statistical variability across wafers, panels, and lots further complicates correlation.
- Enabling long-term autonomous model updates (automatically improving predictive models based on new data) is hindered by noisy data (unwanted signal fluctuations), sensor drift (gradual changes in sensor readings), cross-tool calibration inconsistencies (differences in measurements among tools), and the difficulty of separating measurement artifacts (false features introduced by the measurement process) from true physical variation (actual material differences).

Process-Model-Driven Manufacturing and Yield Optimization

- Yield modeling in heterogeneous integration is inherently complex because yield loss mechanisms compound across die, interconnect, bonding, and substrate layers. Accurately modeling stochastic defect distributions—especially for hybrid bonding and fine-pitch RDL—requires detailed process knowledge often unavailable or proprietary.

- Process variation interactions are nonlinear, making Monte Carlo simulations computationally expensive at the system scale.
- Linking transistor-level variability to package-level stress and alignment variation in a unified framework is challenging. Integrating real-time fab conditions into architecture decisions requires secure data sharing and high-speed simulation infrastructure, which presents organizational and cybersecurity hurdles in addition to technical ones.

Multi-Physics/Scale/Domain Capability

- The primary technical barrier is the strong nonlinear coupling between physical domains. Fully concurrent multi-physics solvers are computationally demanding and often unstable for large 3D systems.
- Multi-scale modeling presents another challenge—accurately bridging nanoscale transistor power density at the die level to centimeter-scale board heat spreading without losing fidelity.
- Combining multi-physics and multi-scale modeling and simulation for concurrent co-design of chiplets (with nanoscale transistors and circuits), packaging, and board is a far greater challenge. High-power AI/HPC systems generate extreme thermal gradients that exceed the limits of current material characterization data.
- Incorporating advanced cooling (microfluidics, vapor chambers) adds fluid dynamics complexity that most semiconductor simulation frameworks are not designed to handle natively. Scalability to full-system simulation within practical runtime limits remains a core obstacle.
- Predicting advanced packaging cost is difficult due to evolving architectures, uncertain yields, limited early-stage data, and complex trade-offs between performance, reliability, and manufacturability. Advanced packaging relies on a complex, globally distributed supply chain that includes foundries, OSATs, substrate vendors, and material suppliers.

High-Precision Failure Reliability Models

(Further details can be found in Chapter 24.)

- Failure mechanisms in advanced packaging are rarely isolated; they are coupled, time-dependent, and workload-sensitive. Hybrid bonding interfaces introduce new degradation pathways for which long-term empirical datasets are lacking.
- Modeling electromigration, thermo-mechanical fatigue, and dielectric breakdown simultaneously requires accurate material models across temperature and stress ranges that are difficult to characterize experimentally.
- Accelerated stress tests may not accurately represent real-world workload conditions, making lifetime extrapolation uncertain. Long-term predictive reliability also depends on field-return data sharing, which is often limited by confidentiality constraints. The central challenge is building reliable predictive models without decades of failure history.
- AI-based reliability models face data scarcity and bias challenges, particularly for rare failure events.

AI-Assisted and Fast Simulations to Support Co-Design

- Training surrogate models requires large volumes of high-fidelity simulation data, which are computationally expensive to generate and may not span the entire design space. Ensuring that AI models generalize beyond their training domain is a significant risk, particularly for novel materials or architecture.

- Multi-objective optimization in heterogeneous integration often involves conflicting constraints (thermal, yield, cost, and so forth), making convergence difficult. Adaptive abstraction techniques must balance speed and accuracy without introducing hidden errors.
- Integrating AI tools into established EDA workflows poses compatibility and validation challenges. Explainability and trust remain major barriers—engineering teams must understand and validate AI-generated design recommendations before adoption.

Digital Twin Integration

- Building a true end-to-end digital twin requires integration of design databases, manufacturing execution systems, metrology outputs, and field performance data, which are typically siloed across organizations and tool ecosystems. Data standardization and interoperability remain unresolved challenges. Maintaining model fidelity while updating parameters dynamically can introduce numerical instability or drift.
- Cybersecurity and IP protection concerns complicated cross-company data sharing, particularly in multi-chiplet ecosystems. Real-time twin updates demand significant computing infrastructure and low-latency data pipelines. Long-term lifecycle twins also require persistent data governance over decades, raising challenges in storage, traceability, and model version control.
- Achieving closed-loop optimization across product generations, therefore, involves both deep technical integration and substantial organizational alignment.

Cross-Cutting Grand Challenges

- Computational scalability for multi-physics, multi-scale, multi-domain systems
- Data standardization and interoperability across tools and organizations
- Secure cross-ecosystem data sharing
- Workforce expertise bridging physics, AI, and manufacturing domains

Overcoming all of these challenges is essential to transitioning heterogeneous integration modeling from an advanced analysis capability to an autonomous, predictive, closed-loop system engineering approach.

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