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Review

The application of multi-scale simulation in advanced electronic packaging

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ABSTRACT

Electronic packaging is an essential branch of electronic engineering that aims to protect electronic, microelectronic, and nanoelectronic systems from environmental conditions. The design of electronic packaging is highly complex and requires the consideration of multi-physics phenomena, such as thermal transport, electromagnetic fields, and mechanical stress. This review presents a comprehensive overview of the multiphysics coupling of electric, magnetic, thermal, mechanical, and fluid fields, which are crucial for assessing the performance and reliability of electronic devices. The recent advancements in multi-scale simulation techniques are also systematically summarized, such as finite element methods at the macroscopic scale, molecular dynamics and density functional theory at the microscopic scale, and particularly machine learning methods for bridging different scales. Additionally, we illustrate how these methods can be applied to study various aspects of electronic packaging, such as material properties, interfacial failure, thermal management, electromigration, and stress analysis. The challenges and the potential applications of multi-scale simulation techniques in electronic packaging are also highlighted. Further, some future directions for multi-scale simulation techniques in electronic packaging are concluded for further investigation.

1. Introduction

Electronic packaging is a specialized field within electronic engineering that revolves around enclosing and safeguarding electronic, microelectronic, and nanoelectronic systems, including integrated circuits, passive devices, and circuit boards, from various forms of mechanical damage, as well as addressing concerns such as cooling, radio frequency noise emission, electrostatic discharge, moisture, and other environmental conditions. Effective electronic packaging significantly influences the performance, reliability, and overall cost of electronic systems. As microsystems continue to undergo continuous miniaturization, performance enhancements, and reliability improvements, there arises a necessity for the development of novel materials and manufacturing techniques. A primary challenge within this domain is thermal management, necessitating the creation of materials with superior thermal conductivity to enable efficient heat dissipation, which must be seamlessly integrated into the manufacturing process. Additionally, organic electronic packaging represents a distinctive subset of electronic packaging, focusing on the utilization of polymer-based systems to encase and safeguard electronic, microelectronic, and nanoelectronic components.

Multiphysics simulation serves as a valuable tool for assessing the performance of electronic devices under the simultaneous influence of interconnected physical fields, including electrical, magnetic, thermal, mechanical, and fluid dynamics. These fields interact across diverse media and temporal and spatial scales. The growing interest in multiphysics coupling within electronic packaging stems from the shift away from conventional silicon (Si)-based semiconductor devices towards emerging wide bandgap (WBG) power semiconductors, such as silicon carbide (SiC) or gallium nitride (GaN). WBG semiconductor devices hold promise for significantly reducing switching times and losses. However, realizing these benefits hinges on the effective packaging and integration of WBG devices into innovative compact solutions [1]. In recent years, several compact design solutions have been proposed, such as semiconductor dies embedded in printed circuit boards (PCB) [2,3], integrated direct bonded copper (DBC) modules, or hybrid structures combining PCB, integrated circuits (ICs), semiconductor and DBCs into a single switching cell [4–8]. It is evident that due to compact designs, critical components are placed in closer proximity to one another, leading to heightened and more pronounced multiphysics coupling effects [9].

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Various partial-differential equations (PDEs) can mathematically describe these multiphysics phenomena, such as thermal transport, electromagnetic fields, mechanical stress, etc. As the complexity of the problem increases, solving these physical and coupling equations becomes more challenging. To achieve a high-fidelity representation of real-world problems, it is usually necessary to consider fine 3D geometries with multi-scales, nonlinear field-dependent material properties, and nonlinear interface conditions simultaneously. With the development of microelectronics technology, the chip structures are becoming more miniaturized and compact, and the integration density of the whole system is increasing. This exponentially increase in complexity places higher demands on advanced electronic packaging technology [1] and related design techniques such as numerical simulation. The early use of numerical simulation methods for exploration and trial-and-error in the design process of packaging technologies, including the selection of material parameters, objects and layout dimensions, can significantly reduce the cost of experimentation. At the macro-scale, finite element methods (FEM) are commonly used to model the packaging structure and evaluate its performance.

Furthermore, atomic simulation techniques such as molecular dynamics (MD) and density functional theory (DFT) have been widely used to reveal the microscopic mechanisms of macroscopic phenomena [2,4]. However, for systems composed of multiple materials, achieving trans-scale simulation is exceedingly challenging. This involves coupling both first-principles calculations, which simulate hundreds of atoms over nanosecond timescales, with finite element calculations, which simulate billions of atoms over millisecond timescales.

2. Multiphysics simulation technology of electronic devices

The main physical fields in electronic packaging encompass electric, magnetic, thermal, humid, and stress fields, which exhibit strong interactions, particularly in modern electronic packaging with compact designs. Consequently, a comprehensive evaluation of these physical fields is essential, taking into account real-world operating conditions, realistic material parameters, and coupled partial differential equation (PDE) models throughout the design, production, and operation phases. Multiphysics simulation plays a pivotal role in assessing performance parameters, investigating failure mechanisms, enhancing reliability, and refining packaging methods for electronic devices. In this section, we delve into the coupling relationships among various physical fields involved in multiphysics modeling of electronic packaging, while also addressing the challenges and limitations associated with such simulations.

2.1. Coupling forms of multiphysics in electronic devices

Fig. 1 illustrates the multiphysics coupling relationships inherent in modeling electronic packaging and subsequent numerical simulations. Electronic devices are influenced by coupled electric-magnetic-thermal-mechanical fields and other operating conditions, often due to applied voltage or current excitations. As a consequence, the electric conductivity and insulation properties of materials fluctuate across time and space, leading to intricate interaction and coupling mechanism [10]. The common problem of current sharing could result from variations in stress, temperature, and structure. To prevent thermal failure in electronic packaging, the electrothermal effect of cell conduction must be taken into account for enough accuracy. Moreover, comprehensive thermal control of each module is also necessary when packing devices. It is vital to examine the internal thermal stress, because the solder layer, lead wire, and other components may experience fatigue failure due to the thermal cycle and power cycle, leading to possible packaging failures such as solder layer cavity, bonding wire falling off, and accelerating the rate of component damage. Electromagnetic interference (EMI) in electronic packaging will also affect the operation of nearby circuits and devices; hence electromagnetic compatibility (EMC) must be taken into account at the beginning of design [11–17]. The internal electromagnetic force of the electronic packaging has less impact than the thermal stress while working under normal conditions. High-frequency or high-current pulses will dramatically increase the transient electromagnetic force, causing the power module to bend [18]. In press-pack electronic packaging, there is a bi-directional coupling relationship between the electric and mechanical field because of the contact resistance, as well as the thermal and mechanical field because of and thermal contact resistance [12].

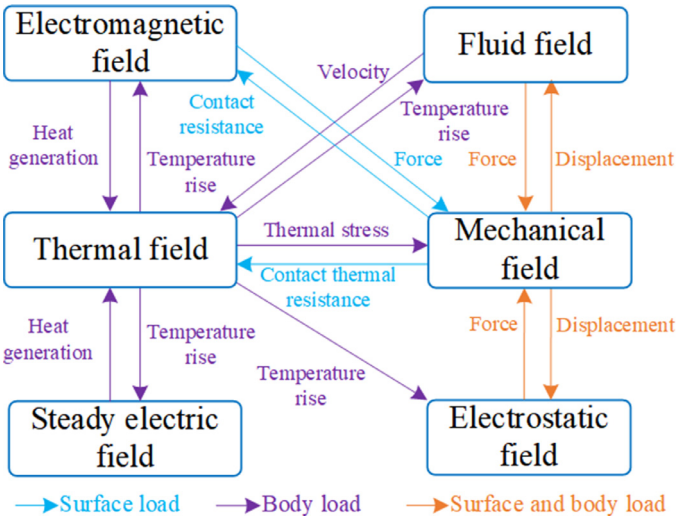

Fig. 1. Interaction of coupled multiphysics including electromagnetic field, thermal field, steady electric field, fluid field, mechanical field, and electrostatic field.

2.2. Characteristics of multiphysics coupling in electronic packaging

The development trends in electronic packaging emphasize compactness, intelligence, high energy, and high current density. Consequently, multiphysics analysis consistently encounters new numerical modeling and computational challenges. The complexity of numerical computations, the demand for accuracy, and the sophistication of design are continuously on the rise. Existing multiphysics coupling models for electronic devices can be categorized into three main types: electric-thermal coupling, electric-thermal-mechanical coupling, and electromagnetic-circuit coupling.

2.2.1. Electric-thermal-mechanical coupling

The electric-thermal-mechanical coupled analysis methods have attracted much attention in research on electronic packaging multiphysics. Fig. 2 shows the coupled electric-thermal-mechanical relationships when used for analyzing single-chip press-pack devices [19]. Establishing an accurate and suitable multiphysics coupling model for numerical computation is crucial for subsequent simulations of various packaging configurations under real working conditions, including excitations or boundary conditions. Key issues in multiphysics simulation encompass the formulation of coupling mechanisms through partial-differential equations (PDEs) or algebraic equations, material constitutive relationship models accounting for the interaction of multiple field intensities, numerical discretization of coupled PDEs and transfer mechanisms, and effective resolution of complex algebraic equation problems [20,21].

The development of packaging technology has been driving electronic packaging design into high frequencies and high power levels [22]. The continuous reduction in circuit feature sizes and the increase in circuit complexities, such as 3D integration, together with the demand for higher frequencies and power levels, present a challenge for the elec-

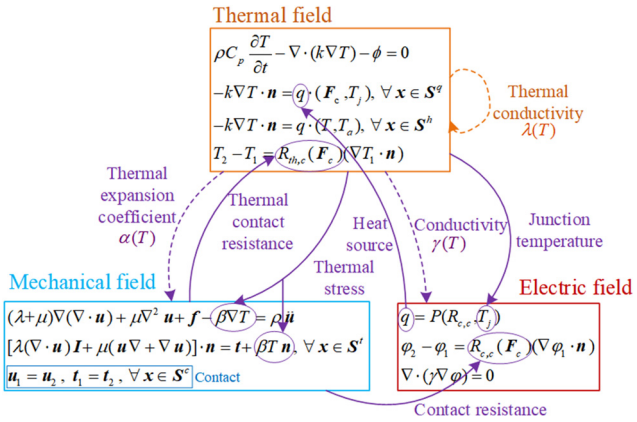

Fig. 2. Multiphysics coupling in electronic packaging.

tronic packaging design: the distribution effect has to be addressed at high frequencies; the thermal effect can no longer be neglected due to the reduced feature size and the increased power levels. Significant temperature rises, especially at hot spots, can degrade the performance and lifespan of electronic packaging and cause metallization failure through electromigration. The induced thermal stress due to large temperature gradients and mismatched thermal-expansion coefficients may lead to mechanical failures, such as delamination and liftoff [23]. Changes in the electromagnetic properties of materials due to high temperatures can result in signal- and power-integrity issues, including clock skew, unintentional voltage drops, and spectrum shifts for filters and resonators. Consequently, a multiphysics-based computer-aided design methodology is required to tackle both electrical and thermal issues simultaneously.

The temperature rise of electronic packaging can be significant globally or high at some local positions if not designed properly, which may greatly affect the electromagnetic properties of the materials used and worsen the performance and quality parameters of the electronic packaging. Therefore, the electromagnetic field analysis has to be coupled with thermal analysis and the computation will be repeated or iterated with updated material properties to quantify the electrical performance, which requires a two-directional or two-way coupling carried out sequentially [24,25]. Despite being a two-way process in the multiphysics modeling of electronic packaging, the electromagnetic-thermal coupling is still a sequential coupling due to significant differences in the temporal variations of the electromagnetic and thermal fields. Two-way simultaneous coupling is only necessary when the temporal variations of the two physical phenomena are of the same order. Usually, the electrical analysis can be performed first, from which the dissipated power can be calculated and used as the heat source to carry out further thermal simulation. Then, the calculated temperature distribution can be used to update the material property parameters for the next simulation cycle. When the electronic packaging or the electronic devices to be simulated are equipped with a fluid cooler, such as microchannels, the electromagnetic-thermal co-simulation can be extended to include fluid analysis to consider the effect of the fluid cooling [26]. With the computed temperature distribution, a mechanical analysis can also be conducted to evaluate the structural integrity of electronic devices. In these multiphysics analyses, coupling can often be simplified as a one-way sequential process because, for most engineering applications, the thermal effect on fluid density and velocity, as well as the mechanical effect on temperature, can be neglected. However, for press-fit electronic devices with contact resistance and thermal contact resistance, electromagnetic-thermal and thermal-mechanical coupling should involve a two-way coupling approach.

In contemporary electronics, insulated gate bipolar transistor (IGBT) modules are extensively utilized, necessitating the development of associated multiphysics modeling methods that cater to a broad application spectrum, including powder modules [27,28]. Several serious failure modes of IGBT modules, such as solder creep, bond wire lift-off/heel cracking, metalization reconstruction, etc., are attributed to thermo-mechanical fatigue. Fatigue is typically induced by time-varying loads, which cause local heating in active components followed by cool-down during passive periods. A common approach for testing the robustness of power module packaging is to simulate the above-mentioned temperature cycling, either through power or passive thermal cycling. In both cases, the test can be replaced with a simulation having real-world conditions, and a power module subjected to the so-called active power cycling [28] is considered. The motivation for the particular case is its resemblance to real-world application. Under these conditions, the dominant failure mechanism observed is bond wire lift-off [29,30]. So far the common approach in degradation and lifetime assessment of IGBT modules failing due to bond wire lift-off has been based on the Coffin–Manson (CM) or CM-Arrhenius model with a parameter corresponding to the load inserted [31,32]. The temperature distribution is often used as load and the model parameters are fitted to accelerated test data by taking shape, environment, degree of damage, etc., into account.

2.2.2. *Electromagnetic field–circuit coupling*

As electronic packaging continues to shrink and operate at higher frequencies, distributive parameters become increasingly crucial compared to lumped circuit parameters for ensuring simulation accuracy. Electromagnetic field-circuit coupled analysis solvers, which combine time-consuming field computation with fast circuit simulation, offer both accuracy and efficiency for practical electromagnetic field analysis of designs. For example, monolithic microwave integrated circuits (MMICs) represent a specialized electronic device category operating at microwave frequencies, fulfilling essential functions such as microwave mixing, power amplification, and high-frequency switching [33]. The MMICs are featured with their distributive components and lumped circuit components, and their design must account for the electromagnetic effects brought on by the mutual coupling of digital electronic devices and the undesirable radiations of the distributive components. Then a full-wave field solver must be used to accurately predict the electromagnetic responses of the integrated and packaged components and systems. The lumped circuit components must, however, be modeled using a circuit solver, such as the one based on modified nodal analysis [34], in case of sufficiently electrically small size. A simple sequential or weak coupling approach is inadequate as it lacks precision and stability, given that the currents and voltages in the lumped circuits vary on a temporal scale similar to that of the fields in the distributive components. To achieve precise and reliable solutions in such scenarios, simultaneous coupling of all field and circuit simulations is essential. This involves solving coupled discrete equation systems that incorporate both field and circuit unknowns together.

There are mainly three ways to couple the electromagnetic field and circuit solvers simultaneously for the modeling of MMICs [35–37]. When the system comprises only a few distributive components, a full-wave analysis can be conducted using an electromagnetic field solver, and equivalent circuits can be extracted for each distributive component. Subsequently, circuit analysis can be employed to obtain the solution for the entire MMIC by incorporating the extracted equivalent circuits for all distributive components. Conversely, if the system primarily consists of a few lumped circuit components, a circuit analysis method can be utilized to determine the admittance of each component. These admittances can then be input into the electromagnetic field solver to solve the entire MMIC. However, both approaches have limitations. The first method overlooks coupling between distributed components, while the second method cannot directly handle active and nonlinear circuit components. The most accurate approach involves solving the coupled electromagnetic and circuit equations simultaneously, coupling the modeling of distributed and lumped circuit components through their interface current or voltage ports.

The electromagnetic field-circuit cosimulation can incorporate multiport distributed or lumped networks, which might have been predesigned and compactly characterized by frequency-dependent multiport network matrices derived from either measurement or simulation. [38,39]. With the extension and incorporation of advanced numerical techniques, such as spatial domain/time decomposition method, flexible temporal time-stepping algorithm, and dispersion modeling in case of wide-band excitations, the electromagnetic field-circuit combined solver can model complicated MMICs and other electromagnetic systems involving nonlinear circuits and complex material properties, such as those encountered in the analysis of integrated antennas, phased arrays, complex electronic systems, and electromagnetic compatibility issues.

3. Challenges for the multiphysics coupling algorithm

The multiphysics analysis of electronic packaging becomes increasingly complex and challenging when addressing nonlinear materials, multi-scale spatial and temporal domains, and strong coupling relationships among fields. The primary issue and ultimate goal for a multiphysics coupling solution are to achieve stable, reliable, fast, and accurate numerical computation. This necessitates a clear and reasonable development of the mathematical model itself, along with a thorough understanding of the fundamentals of the physical process. Research efforts must focus on advanced numerical algorithm optimization to expedite the solution procedure. Significant progress has been made in recent years in this regard. Research on fast algorithms has benefited from the development of novel parallel algorithms, the subdivision of complex models into smaller or locally equivalent ones, adaptive mesh and step size optimization in coupled solutions of various physical fields, and the utilization of isogeometric analysis (IGA).

3.1. Large-scale parallel finite element computation algorithm

As the complexity of engineering problems involving multiphysics grows, so does the computational scale. Additionally, the condition number of the discrete large-scale sparse matrix is often very high in many coupling analyses, making it challenging to efficiently obtain a converged solution using iterative linear solvers. Consequently, sparse parallel direct solvers are gaining popularity in engineering calculations, facilitated by the decreasing cost of computer RAM. A single workstation with sufficient RAM can handle the solution of a sparse matrix with tens of millions of degrees of freedom. For instance, using the sparse direct method solver Paradiso on a Dell Precision T7920 workstation with 1T RAM, one was able to correctly solve a real sparse matrix equation with around 50 million degrees of freedom. Due to the nonlinear complexity of the sparse direct solution technique, it typically grows at the rate of $N\log N$ to N^2, when the degree of freedom reaches tens of millions or hundreds of millions. At this point, it is important to improve the central processing unit (CPU), increase the RAM and disk array, graphics processing unit (GPU), input/output (I/O), and concurrent computing all have upgraded requirements to solve the large matrix system efficiently.

Distributed parallel algorithms or sparse matrix equation algorithms must be taken into account to adapt to a larger solution scale. The growth of numerical techniques, such as parallel computing for large-scale issues, has been facilitated by the evolution of hardware, such as the appearance of multi-core microprocessors. In the absence of an overall coefficient matrix, ref. [40] proposed a parallel algorithm based on the elemental level, where each elemental matrix corresponds to a simplified boundary condition. The element matrix is dispersed throughout the distributed CPU core to aid in the subsequent computation. The overall converged solution can be obtained after a specific iterative process, and the node means the value of the solution is derived by a weighted summation of pertinent nodes. The computing process is substantially accelerated by parallel processing at the cell level. To divide and resolve the discrete linear algebraic equations in numerical computation, the classic parallel approach frequently uses the parallel domain decomposition method or multigrid method. In ref. [41], the finite element tearing and interconnecting (FETI) technique is employed in an electromagnetic field computation to investigate the issues of multiphysics in welded-type electronic device modules, which demonstrated that the computation time can be reduced greatly by employing the proposed technique. The total number of unknowns in a computation can be significantly reduced by employing adaptive techniques, such as refining finite element meshes only in local regions with significant physical gradients. Furthermore, different meshes can be utilized for different physical fields to capture each field's variation accurately.

The complexity of models employed to solve multiphysics problems is expanding exponentially, surpassing the rate at which computer hardware technology is advancing. To effectively and rapidly simulate and optimize large-scale three-dimensional multiphysics of electronic devices, it is imperative to explore innovative numerical approaches and advanced computation techniques.

3.2. Data transfer and step size in the multiphysics coupling computation

Accurate and efficient data transfer among different physical fields is crucial in the coupling. To this end, multi-dimensional data interpolation or fitting techniques like radial basis function (RBF) [42] and fast shell approach [43] have been developed to map nodal data between heterogeneous meshes. The RBF method provides great computation accuracy and is easy to understand and apply. The interpolation impact for nodes with small numerical values is poor when the numerical value fluctuation range is wide, which however is a drawback. Fast shell interpolation can only handle points in convex shells, yet it is effective and versatile.

When employing the finite element weak coupling approach to address electromagnetic-thermal coupling in electronic devices, the metal loss calculated by the electromagnetic field is utilized in the thermal-mechanical fields as a heat source through data transfer. However, the simulation results may deviate from the actual hot spot temperature due to the standard average heat source method, which simplifies the computation of the thermal-mechanical field. The accurate computation of loss density distribution is essential for precise temperature and stress distribution computation. Computational performance may suffer when using a unified fixed mesh, as the sudden increase in the number of elements and degrees of freedom can impact efficiency. Research into nodal data transfer methods among heterogeneous models can address this challenge. Additionally, accurately applying metal loss from the electromagnetic field, considering local non-uniform heat source density, to the thermal-mechanical field can further enhance the solution of temperature and stress distribution. The full electric-thermal-mechanical coupling model and the full thermal-mechanical coupling model based on the finite element approach are established in [12,44]. The electrode plate will warp as a result of the temperature field's effect, resulting in an uneven distribution of stress among submodules of the structure. Then, as a result of the coupling effects of contact resistance and thermal contact resistance, the current density and temperature distribution between the submodules are also uneven, with thermal contact resistance having a greater impact.

The relaxation process of heat transfer or the thermal field is slower to achieve its steady state than that of the electromagnetic field. Utilizing uniform time-step size will thus result in needless repetitive computations of the thermal field when using the finite element approach to solve the sequentially coupled transient electromagnetic-thermal field. Ref. [45] proposed to solve the semi-discrete system with various time steps, and stability analysis uses the time integration approach. The temporal non-uniform step method is used [46] to transfer data at the coupling point of time for each physical field.

3.3. Common methods and key technologies for solving DAEs

Multiphysics simulation often involves spatial discretization of partial differential equations (PDEs) and coupling constraints, resulting in differential-algebraic equations (DAEs) that necessitate further temporal discretization to obtain the final linear algebraic equations. A critical research area in multiphysics computation is the integration of integrators from system dynamics and other disciplines to solve multiphysics problems while ensuring solution accuracy, efficiency, and robustness throughout the computation process. To accurately capture the multiphysics process, the integrator must adaptively track the system's time-varying features and select appropriate time steps. A universal integrator should balance the robust handling of unique problems with the efficiency of addressing common ones [47].

The desired universal DAE integrator should possess the following features. (a) Support variable order integration algorithms and dynamically determine the order and integration step size as needed. (b) Automatically detect discontinuities and instabilities, and adjust the algorithm and solution steps accordingly. (c) Efficient error estimation, allowing for adaptive changes in order and step size while maintaining computational accuracy. (d) Effectively handle numerically-induced non-smoothness in velocity, acceleration, and Lagrange multiplier curves, and automatically restart when the problem cannot be solved at singular configurations. Most commonly used universal DAE integrators employ implicit formats. These algorithms typically include integrator families based on backward difference formula (BDF), integrator families based on implicit Runge-Kutta (IRK) methods, and single-step integrator families with multi-stage or multi-step algorithms.

To solve a differential-algebraic equation (DAE), integrators often encounter the following challenges:

(1) Jacobian matrix-related issues: The Jacobian matrix may become singular or nearly singular under certain configurations of the constrained system. In rigid problems, the Jacobian matrix's condition number can be very large, leading to failed error estimation, reduced computation accuracy, and other numerical issues.

(2) Numerical discontinuities: Computed results frequently exhibit numerical discontinuities due to high-frequency stimulation. The time smoothness of input variables directly impacts the integrator's resilience.

(3) Insufficient satisfaction of implicit constraints: Implicit constraints are often inadequately satisfied during the simulation process. Spikes in the Lagrange multiplier curve are a common example of evident discontinuities, making numerical computations challenging.

(4) Inaccurate step size estimation: In various non-smooth situations, step size estimation may be inaccurate, resulting in large computation errors and an increase in overall computation requirements.

In addition to the direct method mentioned above, converting a DAE into an ordinary differential equation (ODE) and utilizing an ODE integrator for simulation is a widely-used technique. However, commercial software is rarely employed in practice for this technique due to its low processing efficiency and weak robustness. When the restricted equations are sufficiently smooth, the Baumgarte reduced order technique can also yield accurate results. Other lower-order techniques either apply the modified dynamic equations [48,49] pull back with the penalty function, or choose the penalty factor in conjunction with the integration step [50]. High-frequency degrees of freedom are typically introduced by these reduced-order approaches. At this point, rigid integrators or specific explicit integrators are required to assist with the solution [51,52].

3.4. Integrated CAD/CAE isogeometric analysis technique

The finite element method is encountering demands for enhanced spatial discretization effectiveness and the quality of mesh generation, driven by the intricate geometry and material composition of electronic packaging. Integrating the analytical model and geometric model can significantly enhance the effectiveness and precision of the numerical model, while also circumventing the time-consuming mesh generation process and frequent interaction of data during mesh refinement. To address these challenges, spline theory-based isogeometric analysis (IGA) is proposed [53]. To achieve the mapping from the spline model parameter domain to the physical model, isogeometric analysis (IGA) utilizes a precise geometric model in a computer-aided design (CAD) system. This approach allows for a unified expression between the geometric model and the analytical model, eliminating the need for secondary modeling of numerical computations and reducing the time required for frequent interactions with the geometric model during the mesh refinement process. IGA offers several advantages in solving large-scale and complex engineering problems, including high-precision geometric modeling, straightforward mesh generation and refinement, and high-order continuity. The IGA technique can circumvent the computation inaccuracy associated with polynomial approximation expressions and achieve computation accuracy comparable to finite element method (FEM) with fewer degrees of freedom.

Non-uniform rational B-spline (NURBS) is used as the basis function in the IGA. Because the NURBS basis function can attain continuity on the element's boundary, improving the smoothness can improve the accuracy of the numerical solution [54,55]. A new method of numerical computation has been created based on the IGA. For instance, the iterative technique is employed to solve a large algebraic equation produced by IGA when the cost of direct computation is too high. Ref. [56] proposed a multigrid conjugate gradient approach appropriate for IGA. The conjugate gradient is used in the basic iterative technique, while multigrid is used in the pretreatment. The method has the advantages of both the conjugate gradient method and the multigrid method. Due to the increase in NURBS basis function order in multigrid, the error with sluggish attenuation can be rapidly attenuated in the conjugate gradient approach. Ref. [57] proposed the IGA boundary element method (IGABEM), the boundary of the model is discretized using the boundary element approach for the thermal analysis of electronic device substrates, and the problem's dimension is reduced to a large extent.

4. Single-scale simulation method for electronic packaging

Numerous factors in advanced packages and heterogeneous systems can push the stress to the limits compared to traditional packages. Therefore, to predict reliability, mechanical modeling should be considered early in the design. Finite element mechanical modeling has been widely used to predict phenomena such as interconnect (solder joints, etc.) stress, and stress in through silicon vias (TSVs). There are several typical issues in mechanical simulation in electronic packaging, such as multi-scales from millimeter to the micrometer, topological evolution due to interfacial delamination/crack propagation, etc.

The development of microelectronics technology has been promoting the development of chips toward smaller structures and higher integration density, and its complexity is increasing exponentially, which puts forward higher requirements for advanced electronic packaging technology [58]. At the macroscopic scale, the device and packaging structure is typically modeled and calculated using the finite element method (FEM) thanks to its versatility for being capable of treating complex geometry, material composition and all kinds of loads or excitations. To include further details and physical laws, atomic simulation techniques such as molecular dynamics (MD) and density functional theory (DFT) are also widely used to reveal the microscopic mechanisms of macroscopic phenomena [59,60]. However, it is still extremely challenging to realize the trans-scale simulation by combining first-principle calculations with finite element calculations. In summary, the simulation of electronic packaging is mainly based on first-principle methods for simulation at the microscopic level, the MD method for simulation at the microscopic and mesoscopic levels, and the FEM for simulation at the mesoscopic and macroscopic levels.

4.1. DFT-based first principle simulations

First-principles computational simulation method is an algorithm that directly solves the Schrödinger equation after some approximation processing based on the principle of the interaction between the nucleus and the electron and its basic laws of motion, using the principles of quantum mechanics [61,62]. This method starts from the scale of atoms and electrons that constitute the most basic unit of matter to recognize the properties of matter. Density functional theory (DFT) overcomes the complexity of the Schrödinger equation by replacing the wave function with electron density as the basic quantity [63–65]. The DFT theory originated from the Thomas-Fermi model proposed by Thomas and Fermi based on the assumption of a uniform electron gas in an ideal state and was gradually improved with the Hohenberg-Kohn theorem and the Kohn-Sham equation [63,66]. DFT-based first principle calculation can be used to calculate electronic structures (energy bands, density of states, charge density, etc.), mechanical properties (elastic constant, elastic modulus, etc.), thermodynamic properties (formation energy, surface energy, adsorption energy, etc.) and kinetic properties (reaction energy barriers, etc. [67]). At present, the popular first principle calculation software includes Vienna Ab initio Simulation Package (VASP) [68,69], Cambridge Sequential Total Energy Package (CASTEP) [70], Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization (Quantum ESPRESSO) [71], CP2K [72], and Gaussian [73], etc.

Various types of research have been conducted on electronic packaging-related topics using first-principles calculations and the DFT framework. Zheng Tang et al. [74] used DFT theory to simulate the dielectric constants of three typical polymer materials polyethylene (PE), polytetrafluoroethylene (PTFE), and polystyrene (PS), and the results were in good agreement with the experimental data. They demonstrate the feasibility of the DFT method in screening low dielectric constant polymer materials for potential electronic packaging. Cui Zhen et al. [75] used DFT-based first principle calculations to investigate the effect of silicon molecules on pristine and hydrolyzed $CaAlSiN_3$ [010] at the atomic level. $CaAlSiN_3$:Eu^{2+} red phosphors and their organosilicon/phosphor composites are considered to be very promising materials for high color rendering white light-emitting diode (LED) packaging materials [76].

4.2. MD simulations

MD is an important computational simulation method for solving many-body problems at the atomic and molecular levels and is thus used to predict the dynamic properties of nanoscale materials [77]. Using Newton's laws of motion to solve the equation of motion, the trajectory of the atom on the potential energy surface can be obtained. In a certain period, by simulating the motion state of molecules and atoms in the system, the behavior of the system evolving with time can be observed dynamically. To distinguish from the potential function used, MD is mainly divided into ab initio molecular dynamics (AIMD) based on DFT, classical MD based on empirical potential functions, and MD based on machine learning potential functions. MD simulation software currently mainly includes GROMACS [78], CHARMM [79], AMBER [80], NAMD [81], and LAMMPS [82].

Haibo Fan et al. [83] used the MD simulation method to study the interfacial failure of electronic packaging materials under thermal cycling conditions at the molecular level. By calculating the interfacial energy of the epoxy molding compound (EMC) cuprous oxide system during the thermal cycle test, the analysis shows that the cuprous oxide content in the copper substrate has a great influence on the interfacial adhesion between EMC and copper, which is consistent with the experimental observations. To study the coalescence kinetics of nano-copper particles in wide-bandgap semiconductor packaging technology, Xu Liu et al. [84] used the MD method to simulate the rotational behavior, microstructure, and dislocation distribution of nanoparticles of different sizes. They investigated the effect of copper particle size on the sintering process and coalescence mechanism, as shown in Fig. 3. Hu Dong et al. [85] used LAMMPS to realize reactive force field (ReaxFF) MD simulations of sintered silver nanoparticles in electronic packaging in extreme environments (high temperature, high humidity, and high sulfur). Visual analysis of this atomic-scale sulfidation process shows that the formation of the sulfide layer is formed by the upward migration of silver atoms.

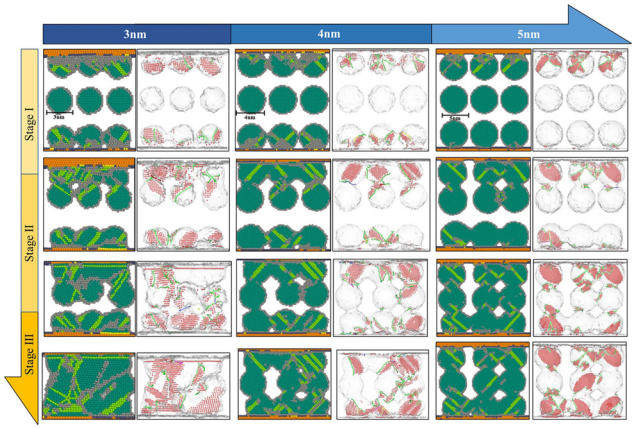

Fig. 3. Microstructure of Cu with different grain sizes during sintering [29].

4.3. FEM simulations

4.3.1. Modeling techniques in FEM

The sub-modeling technology makes the original rough meshing finer by interpolating the solution of the initial global model; this technique is to study the local part of the model. The sub-modeling technique is very effective when it is necessary to obtain an accurate solution for a local part of the overall model if the modeling of this local region has little effect on the solution of the overall model.

The sub-model runs as a separate analysis of the global analysis. The sub-model is a single analysis that can be used at any number of levels. For subsequent sub-models, the sub-model can also act as a global model. The results of the global model are interpolated to nodes on the appropriate part of the sub-model boundary.

Modeling and simulation tools are capable of simulating the mechanical behavior of the package under various environmental conditions such as temperature, vibration, shock, and so on. Sub-modeling techniques can be used to transfer results from the system (board) level domain to chip-level structures, as shown in Fig 4. However, these functions often do not have accurate models for key failure modes, which are important in 3D heterogeneous systems [86].

Adaptive meshing is a mesh that allows the mesh to move independently of the material, maintaining a high-quality mesh throughout the analysis even if the material loss occurs. Adaptive remeshing is mostly used for precision control, while it can also be used for distortion control in rare cases. The goal of adaptive re-meshing is to obtain a solution that satisfies the set mesh discretization error metric goal while minimizing the number of elements, thereby reducing the cost of analysis.

Coupled field analysis, also known as multiphysics analysis, is an analysis that combines different disciplines (physics). For global engineering problems, coupled fields can be used for analysis, and the interaction between different disciplines can handle the problem well. The analysis is coupled when the input of one field analysis is related to the results of another analysis.

Some analyses may have one-way coupling. In some problems, it is not necessary to iterate between the two field solutions. Another more complex case involves two-way coupling. Bidirectional coupling prob-

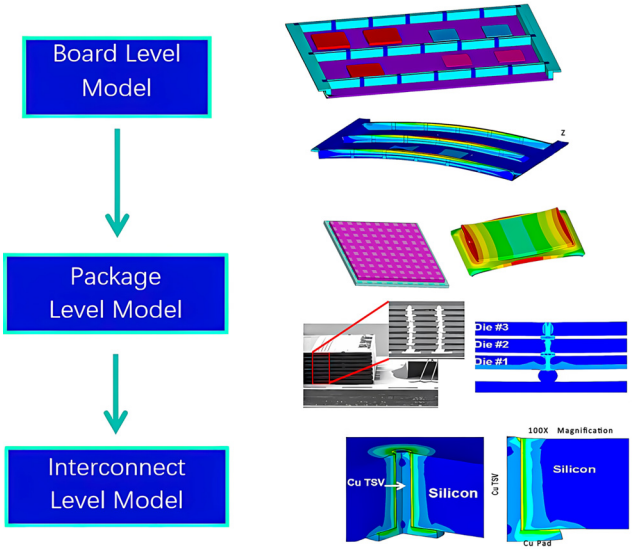

Fig. 4. Mechanical (Vibration) chip-package-board design. Pictures are reproduced [86].

lems require iteration between the two physics to achieve convergence. For heterogeneous systems, modeling must be multiphysics, which will involve one-way or two-way coupling of related physics. For example, in a fluid-structure interaction problem, fluid pressure causes structural deformation, which in turn leads to changes in the fluid solution. This problem is a two-way coupling problem and requires iteration between the two fields.

For heterogeneous systems, there are various load conditions such as thermal load, humidity load, and mechanical load. Therefore, the modeling must be multiphysics, which will involve one-way coupling or two-way coupling of related physics [87,88]. Coupling between fields can be achieved by direct or indirect (load transfer) coupling. Different fields may be solvers for different types of analyses. Therefore, during the simulation, this can lead to complex coupling between fields.

Most mechanical simulations do not consider the effects of transient and steady-state temperature gradients but only focus on thermal stress caused by the thermal mismatch. Some moisture-sensitive materials [89], such as polymer materials, swell during moisture absorption and shrink during desorption. Additional mechanical stress is induced during this process.

Electromigration, an enhanced mass transport process in current-carrying metals induced by a driving force generated by an electric field [90], is one of the key reliability issues in electronic devices. The formulation and solution of this electromigration-coupled physics problem have been studied for decades. However, according to the existing literature, the solutions to the electromigration problem are not consistent. Recently, newly developed models by Cui et al. [88] fully couple these physics fields in a self-consistent and complete manner, proposing concentration-based failure criteria. The implementation of this multiphysics model has been done using ANSYS [88].

The accurate simulation and modeling of electromigration are immature, and the accuracy of electromigration modeling is still vulnerable to various problems. For example, the use of electromigration modeling is not appropriate when one fails to address the coupling relationship between concentration and mechanical stress. For nanoscale interconnects used in CMOS processes, electromigration is highly dependent on the microstructure, bond strength, and interface material structure. Traditional finite element-based modeling has been unable to meet the requirements of S&M for electromigration. To accurately predict electromigration failures, nanoscale modeling approaches are inevitably required.

4.3.2. Challenges and solutions

The main challenges of mechanical modeling lie in the following areas:

(1) New materials exhibit highly nonlinear and unconventional behavioral complexity.

(2) Uncertainty, higher complexity, and variability in the manufacturing process lead to random and complex behavior in the system.

(3) Develop efficient simulation tools that can handle modeling at multiple levels, from chips and packages to boards and systems.

For mechanical problems, new numerical methods are needed to solve them. However, the model step-down method still has limitations, which are difficult to solve for the highly nonlinear behavior of materials.

Accurate material data and characterization of heterogeneous systems are critical, so it is important to establish greater linkages between metrology and stress and multiphysics models. Further work is required to convert the data from metrology to modeling tools, as shown in Fig. 5.

The stress and damage depend on multiphysics loads, which need to be addressed in modeling tools. To predict the electrical-thermal-chemical-mechanical properties of chip package board systems, full synergistic simulations are required. At present, there are some analysis tools and designers performing stress analysis at the mold, chip, packaging, and system levels which need to be improved.

EDA companies offer logical, physical, and electrical design systems, but little integration of stress analysis. There is a tighter integration and co-design of stress at the device, package, board, and system levels. Stress analysis of individual components without capturing system effects and constraints is not feasible for heterogeneous systems. Continued research is needed to improve multiphysics and multiscale modeling tools.

4.4. Hybrid simulations

Many studies of electronic packaging materials have adopted the concept of hybrid simulation, they did not use only DFT, MD, or FEM in their research, but a combination of different simulation methods. To be clear, hybrid simulations are different from multiscale simulations in that they are not transferable in terms of models, but simply study different properties using different methods.

Yuqin Zeng et al. [91] used a combination of MD simulations and first-principles calculation to study the properties of graphene/epoxy electronic packaging composites. Firstly, the molecular dynamics models and first-principles calculation models of epoxy resin, graphene/epoxy resin, and graphene oxide/epoxy resin composites were constructed. The interaction between graphene, graphene oxide, and epoxy resin was obtained by molecular dynamics, and the distribution state of graphene, graphene oxide, and epoxy resin molecules at different temperatures was studied and analyzed by the radial distribution function. Then, physical quantities such as atomic spacing, total charge density, differential charge density, the density of states, formation energy, and charge transfer are obtained using first-principles calculation. The surface-interface interaction between graphene, graphene oxide, and epoxy resin was studied, and the composite mechanism between graphene, graphene oxide, and epoxy resin was revealed. The bonding stability between graphene, graphene oxide, and epoxy resin was also analyzed.

Rong An et al. [92,93] established the initial configuration of the intermetallic compound in the electronic packaging solder joint at the atomic scale by the first-principles method and calculated the basic physical properties such as crystal structure, equation of state, Debye temperature, thermal conductivity, etc. Then, by applying different deformations to the IMC crystal, the elastic properties of single crystals are obtained, the elastic properties of polycrystals are deduced based on VRH and HS theories, and the mechanical anisotropy is analyzed, and the ductility and brittleness are discussed at the same time. Further, based on the Tersoff-Brenner bond level potential model, they es-

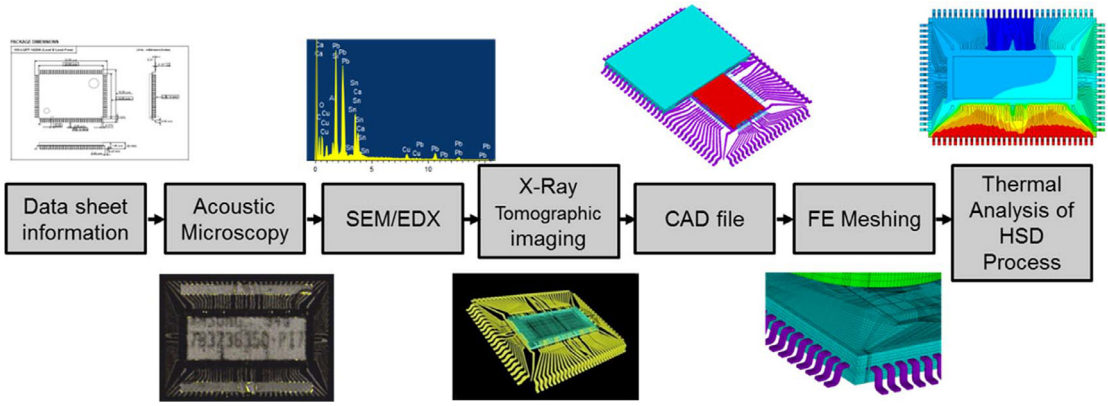

Fig. 5. Integrating metrology with modeling. Pictures are from ref. [86].

tablished the interaction potential for Sn atoms and combined MD to predict the crystal structure, binding energy, bond distance, and bond energy of β-Sn and α-Sn. The α-Sn and β-Sn crystal vibrational mode densities and heat capacities were calculated, and the $\alpha \leftrightarrow \beta$ phase transition of Sn was studied [94].

Yue Zhang et al. [95] used a combination of MD simulation and FEM simulation to study the moisture absorption failure behavior of two typical plastic electronic packaging components, Plastic Ball Grid Array Package (PBGA) and Plastic Quad Flat Package (PQFP). MD simulations were used to calculate the diffusion coefficient of water molecules under different conditions, and the results showed that the diffusion coefficient increased with increasing temperature and decreased with increasing water content in the epoxy resin. At the same time, it was also found that the main way for water molecules to diffuse into plastic electronic packaging devices is diffusion along interfaces or gaps. They then modeled the PBGA using FEM simulations to simulate the stress distribution as the device absorbs moisture. Simulations show that the damp thermal stress in plastic packaged devices is mainly caused by the mismatch of the expansion coefficients of various materials in the device [96].

To study the mechanism of ultrasonic wire bonding in electronic packaging, Yong Ding et al. [97] used FEM to analyze the elastic-plastic deformation during the ultrasonic wire bonding process and determined that the maximum contact pressure always appeared at the periphery of the contact interface. Then, based on this conclusion, a two-dimensional atomic model was established, and the Sutton-Chen potential energy function was used for MD simulation to study the microscopic mechanism of ultrasonic wire bonding, that is, the strong interatomic force in the close contact between the gold wire and the pad led to the interface bonding. At the same time, a method for estimating the interface welding strength of ultrasonic wire welding was proposed based on the results of FEM and MD [98].

5. Multi-scale simulation methods for electronic packaging

Different from the previous hybrid simulation, the multiscale simulation method can achieve simulation accuracy and model transferability. It can realize the continuous simulation of the same system from microscopic to mesoscopic and then to macroscopic and can not only obtain physical properties but also study its internal mechanism. Multiscale simulation methods are of great significance for the study of electronic packaging, but little related research has been reported. The methods that are expected to achieve multi-scale simulations are described below.

5.1. Multi-scale simulation from DFT to MD

As stated above, first-principles calculations based on DFT theory and MD calculations based on empirical potential functions are widely used to study electronic packaging materials, but these studies have not achieved true multi-scale simulations. First-principles studies using DFT and AIMD are very effective in predicting mechanical, electronic, and optical properties of materials [99–101]. Nonetheless, the computational cost increases dramatically with decreasing crystal symmetry and increasing unit cell size, which limits the timescale and size of AIMD to hundreds of atoms and a time within 100 ps [102]. For applications with larger size unit cells and longer simulation times, MD simulations are not available.

A key factor in MD simulations is the force field or interatomic potential [103]. They define the interactions of atoms in the system, and the accuracy of the results depends on the choice of these potential functions. These mathematical functions are fitted to reference data based on the material physical properties of a specific species or compound and a set of specific properties. These potential functions are generated within a specific range of composition, temperature, and structure for a specific material, and results outside that range may be meaningless. Current MD simulations mainly rely on empirical force fields such as EAM potential and LJ potential, but the accuracy and transferability of these models are often questionable [104–106].

Machine learning (ML) methods are used to bridge the simulation across scales to achieve more accurate simulations. ML is a method of using known data, training a model, mining the internal implicit relationship, and then using the model to make predictions. As the core of artificial intelligence (AI), ML is widely used to solve complex problems in engineering applications and scientific fields, such as autonomous driving, geological exploration, information recognition, and medical diagnosis [107,108].

As mentioned earlier, the ML interatomic potential can be used as an alternative to the empirical potential for MD simulations. The advantages of ML interatomic potential applied to MD simulations are mainly in three aspects. First, the dataset of ML interatomic potentials is calculated by first-principles calculations based on DFT (e.g., AIMD), making its accuracy comparable to DFT. Meanwhile, MD simulations using ML interatomic potentials are consistent with classical MD simulations in simulated model size and time scale. Finally, by modifying the source code of the MD software, it can directly use the ML interatomic potential function, which greatly accelerates the MD research process.

The generation methods of these interatomic potentials are similar in principle. First, the original dataset needs to be constructed using first-principles computational software packages (VASP, Quantum ESPRESSO, CP2K, etc.). The atomic coordinates, atomic types, interatomic potential energy, and interatomic forces of the system in the data samples to construct training datasets and test datasets. Then the processing methods are used to determine the ML descriptors to ensure that the model can meet certain physical common sense, such as the potential energy of the same atomic structure remains unchanged after

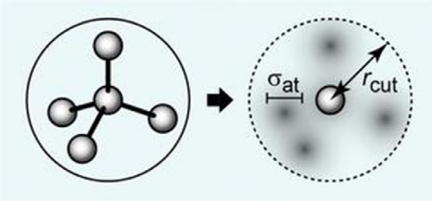

Fig. 6. The sketch map of the SOAP representation.

translation or rotation. The main difference between these methods is the regression algorithm, which is applied to map the descriptors to the potential energy.

There are many promising machine-learning-based interatomic potential methods developed recently, mainly including Gaussian approximation potential (GAP) [109], deep potential molecular dynamics (DeePMD) [110], fast learning of atomistic rare events (FLARE) [111], and proposed physically informed neural network (PINN). Each of them has its pros and cons. The six commonly used methods, that cover most of the characteristics of the machine-learning-based interatomic potential methods, are discussed here to show how to use ML to generate the interatomic potentials and their superiority.

5.1.1. GAP

GAP is a Gaussian kernel-based method applied to generate the interatomic potential. In this approach, the 4D sphere is extended using the predetermined coefficients to represent the atomic environment in a bispectrum space. The configurations from two adjacent atoms or one atom during the two sequential MD steps are strongly correlated. Here, the random sampling method, a sparsification procedure, is used in GAP to solve the problem. The smooth overlap of atomic positions (SOAP) is a many-body descriptor, that is adopted with the GAP model to predict molecular properties [109]. Within SOAP, Gaussian functions are applied to the atoms inside the cutoff sphere, r_cut, with the smoothness controlled by the variance of the Gaussian, σ_at, as shown in Fig. 6. The kernel function is used to measure the similarity between different environments, which directly impacts the accuracy of the GAP model.

5.1.2. DeePMD

DeePMD is an interatomic potential function fitting method, which simulates the relationship between the sum of atomic energy and all atomic environments through the deep neural network (DNN) [110]. DeepMD is carried out by the DeePMD-kit software, and its main workflow is shown in Fig. 7. More specifically, based on the principles of DeePMD, a workflow method is proposed for automatically generating ML interatomic potentials, called DP-GEN [112]. DP-GEN independently explores the initial structure, generates data sets through quantum computing software packages such as VASP, uses DeePMD-kit to train ML interatomic potentials, and then verifies the accuracy of potential functions with MD computing software such as LAMMPS. This automatic looping workflow greatly improves the efficiency of potential function training. At present, DeePMD has been applied to various material systems, such as elemental systems, multi-component systems, water-related systems, molecular systems and clusters, and low-dimensional systems [113]. The MD simulation using the DeePMD interatomic potential has achieved a simulation of 100 million atoms with *ab initio* accuracy and has won the 2020 Gordon Bell Prize for this [114].

5.1.3. FLARE

FLARE is an active learning, one branch of ML, potential generating method based on the Gaussian process (GP). Unlike other methods, (1) FLARE predicts a distribution of energy or force, not a single value; (2) the GP model is trained during the AIMD process, rather than after that. The workflow of FLARE is shown in Fig 8. First, the DFT calculation is called with arbitrary structure as input, and then the GP regression model is initialized with the results of the DFT calculation. After that, the forces on all atoms are predicted through the GP model. If the uncertainty of the forces predicted by GP is lower than the threshold, the results predicted by the regression model will be adopted as the next MD step; otherwise, the DFT calculation will be called and the local environment with the highest uncertainty will be added to the training set to update the parameters of the GP model. Based on the workflow,

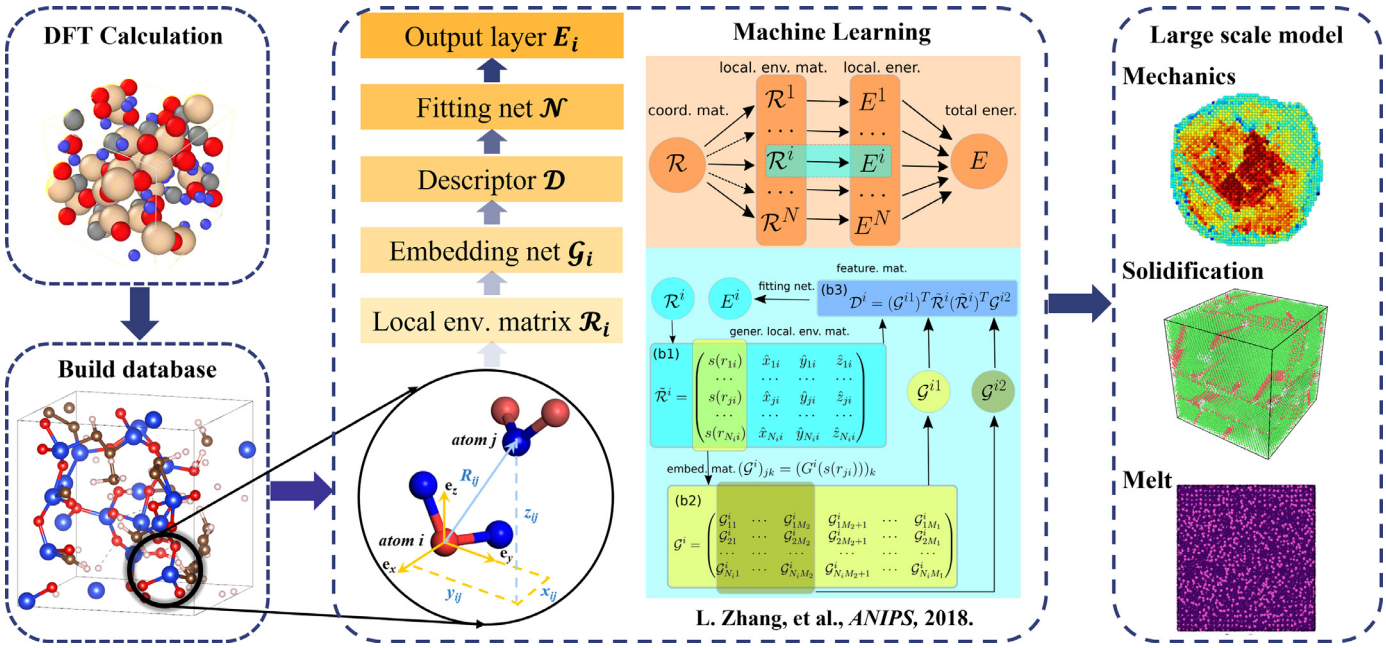

Fig. 7. Schematic plot of the DeePMD-kit architecture and the workflow. The gray arrows present the workflow. The data, including energy, force, virial, box, and type, are passed from the Data Generator to the DeePMD-kit Train/Test module to perform training. After training, the DeePMD model is passed to the DeePMD-kit MD support module to perform MD. The TensorFlow and DeePMD-kit libraries are used for supporting different calculations. See text for detailed descriptions. [110].

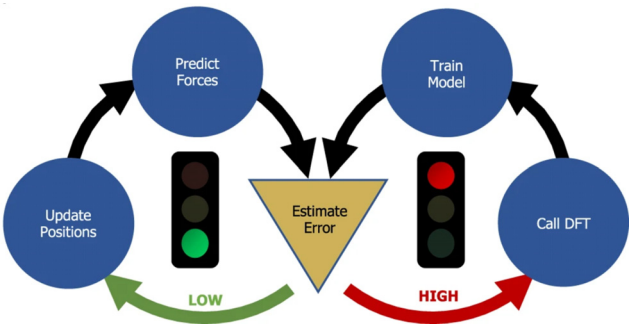

Fig. 8. The framework of the FLARE algorithm. Left loop: If the estimate error is lower than the threshold, MD steps are performed using the current GP force field. Right loop: If the estimate error is higher than the threshold, DFT is called and the GP force field is trained by the DFT data with the highest uncertainty local environments [111].

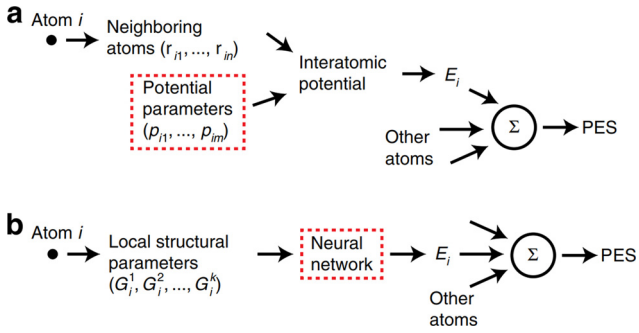

Fig. 9. Flowcharts of different atomistic potentials. (a) Mathematical NN potential. (b) PINN potential.

the ML potential is generated by the continuous iteration of the above process. Fewer DFT calculations are required to capture unexplored configurations, such as defects that exhibit high uncertainty, which can lead to the discovery of unusual phase transition mechanisms in 2Dstanene [111].

The generation methods of these interatomic potentials are similar in principle. First, the original dataset needs to be constructed using first-principles computational software packages (VASP, Quantum ESPRESSO, CP2K, etc.). The atomic coordinates, atomic types, interatomic potential energy, and interatomic forces of the system in the data samples are arranged to construct training datasets and test datasets. Then the processing methods are used to determine the ML descriptors to ensure that the model can meet certain physical common sense, such as the potential energy of the same atomic structure remains unchanged after translation or rotation. The main difference between these methods is the regression algorithm, which is applied to map the descriptors to the potential energy.

5.1.4. PINN

Since the structure-energy mapping is not guided by any physics or chemistry, the regression only ensures accurate numerical interpolation between the DFT points. Extrapolation outside the domain of known environments is purely mathematical and thus cannot be expected to make physically meaningful predictions. Thus, the development of general-purpose type ML potentials suffers from the lack of physics-based transferability presented.

The recent PINN model aims to improve the transferability of ML potentials by integrating an NN regression with a physics-based interatomic potential. As shown in Fig. 9b, the mathematical NN potentials methods directly map $G_i^l \mapsto E_i$, where G denotes the representation of the local structural information. To improve the transferability of interatomic potentials to unexplored atomic environments, PINN adds an intermediate step: $G_i^l \mapsto p_i \mapsto E_i$.

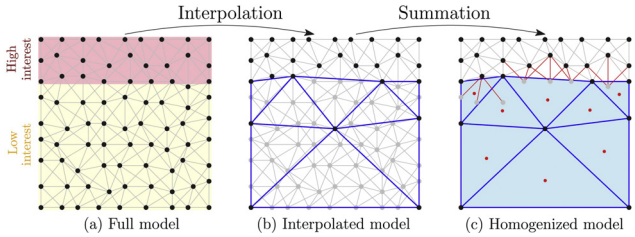

Fig. 10. The principle of QC method: all atoms near the high-interest region are represented, while the deformation of the low-interest region is more uniform, and the atomic density is reduced by interpolation. (a) Full network of nodes (black) and links (gray) with denoted areas of low (yellow) and high (ping) interest; (b) interpolated model with rep nodes (black circles), hanging nodes (gray circles), and interpolation elements (blue triangles), all gray links are evaluated explicitly; (c) simplified model with homogenized material (light blue), sampling points (red circles), and links modeled explicitly in area of high interest (gray lines) and on the interface (red lines) [59].

The first step is executed by the NN and the second by a physics-based interatomic potential. Fig. 9d is a trick to improve the computational efficiency by dividing the parameters into two subsets: local parameters $a_i = (a_{i1}, \ldots, a_{i\lambda})$ and global parameters $b = (b_1, \ldots, b_\mu)$.

The ML-based interatomic potentials have been widely used in many different domains, such as elements, alloys, phase change materials, energetic materials, and defects for their superiority of accuracy and cost compared with AIMD and classical MD. Thus, the ML-based potential would be a promising candidate for the large-scale simulation of electronic packaging.

5.2. Multi-scale simulation from MD to FEM

The combination of MD and FEM is a key step for multiscale simulation to move to the macroscale. The main problem of implementation is the coupling of the model from the atomic level to the continuum, and several methods have been developed. The original idea of combining MD and FEM is to directly combine MD and FEM. In the bonding area between atoms and finite elements, atoms and nodes correspond one-to-one and directly convert atomic forces into concentrated loads acting on finite element nodes. There are many shortcomings in this method, so Finite Element-Atomistic (FEAt), quasicontinuum (QC), macro atomistic ab-initio dynamics (MAAD), and coarse-grained molecular dynamics (CGMD) methods are developed on this basis.

The FEAt method was proposed by Kohlhoff et al. [115], and its principle is to divide the entire model into four components, where the first three areas are for the MD simulation region, and the last three areas are for the FEM simulation region. The two areas in the middle are transition regions, which are described by non-local elastic theory. The biggest feature is that the stress at one point x in the region is related to the strain at all other points x' in the element. The elastic constant in a continuum is defined by the potential energy function between atoms. This method combines discrete and continuous quantities and is applied to simulate some simple crystals.

The QC method was proposed by Tadmor and Ortiz et al. [116], whose principle is different from that of FEAt. This method no longer uses a specific transition region to connect the atomic region and the continuous region. The QC method considers that in some regions of the atomic system where the deformation gradient is relatively smooth, it is not necessary to perform MD calculations on all atoms. Therefore, it only selects some representative atoms to obtain the displacement by MD calculation, and the displacement of other atoms is calculated by the linear interpolation principle in FEM, as is shown in Fig. 10. The computational process of the QC method is both accurate and simple, and

has been widely used in the study of structural failure, micro-defects, and crack propagation[117–121].

The MAAD method is a multi-scale simulation method proposed by Abraham et al. [122] to study the crack fracture process of silicon. Its characteristic is that the method not only combines MD and FEM, but also uses a tight-binding model (TB) based on quantum mechanics theory at the fracture to simulate the breaking process of atomic bonds. MAAD is the closest approach to realizing a multiscale simulation process from first-principles calculations to MD to FEM. This method adopts the idea of a transition region similar to FEAt, and the total energy of the whole system (HFEM, HMD, HFEM/MD, HTB, HMD/TB) is composed of the sum of the energy of each region. The energy of the transition region (HFEM/MD, HMD/TB) is determined by a linear combination of energy functions on both sides of the region, and the combination coefficient depends on the respective energy contributions to the transition region. MADD shrinks FEM cells down to the atomic level, which improves accuracy but limits model size and timescale.

The CGMD method was proposed by Rudd and Broughton et al. [123]. Its basic idea is to play a leading role in the MD simulation of key areas that require detailed calculation, and FEM simulation is used in the parts far from the key areas. In principle, CGMD is similar to the QC method, but it solves the problem that the temperature cannot be considered in the QC method. In the process of practical application, the roughening energy formula is not easy to calculate, which limits its application.

The method of coupling MD and FEM has not been applied to study electronic packaging, but it has been used to study the mechanical properties of single crystals [124], the thermomechanical response of polymers [125], and the strength of structural steel welds [126], etc.

6. Conclusion

The research on multi-scale simulation in advanced electronic packaging has made significant progress in recent years. These approaches have proven to be a valuable tool in predicting the behavior and reliability of electronic devices, thus has enabled the design of more efficient and cost-effective packaging solutions. However, there are still several challenges that need to be addressed to further advance this field. The effectiveness of multi-scale simulation in electronic packaging is dependent on various factors such as material properties, environmental conditions, and simulation models. To improve the accuracy and reliability of simulation results, future efforts should focus on developing more accurate material models, incorporating more comprehensive environmental conditions, and validating simulation results through experiments. Furthermore, the application of multi-scale simulation in electronic packaging is still limited by computational resources and time. Therefore, the development of more efficient and parallelizable simulation algorithms, as well as the use of high-performance computing resources, will be essential for further progress in this field. In summary, although the application of multi-scale simulation in advanced electronic packaging has shown promising results, there are still several challenges that need to be addressed to fully exploit its potential. Future efforts should focus on the following aspects:

1. Development of more accurate and efficient multi-physics models for electronic packaging, taking into account the strong nonlinear and coupling relationships between different physical fields.

2. Further exploration and optimization of various algorithms, methods, and computational techniques to settle the issues faced in multi-physics modeling.

3. Integration of ML methods into multi-scale simulation to enhance the accuracy and efficiency of electronic packaging modeling.

4. Investigation of the impact of different materials and structures on the performance of electronic devices, and the optimization of electronic packaging design to achieve better performance.

5. Collaboration between experimental and simulation researchers to obtain more accurate data and validate the simulation results.

6. Exploration of the impact of more environmental factors such as temperature, humidity, and radiation on electronic packaging performance.

7. Investigation of the aging of electronic packaging and its impact on device performance, and the development of strategies for extending the lifetime of electronic devices.

Declaration of competing interest

The authors declare that they have no conflicts of interest in this work.

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