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Thermomechanical Reliability and Interface Engineering of Polymers in Advanced Semiconductor Packaging

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Abstract. Advanced semiconductor packaging increasingly relies on polymer dielectrics, epoxy molding compounds (EMCs), and underfills for insulation, encapsulation, stress redistribution, and interface protection. This narrative review considers these materials through their application-specific performance envelopes and links formulation and process history to package deformation and local failure. Coefficient of thermal expansion (CTE) mismatch, E(T,t), glass transition temperature (Tg), cure shrinkage, geometry, moisture uptake, and interface chemistry together govern residual stress, warpage, energy release rate, crack growth, delamination, and lifetime. Common design rules are context-depedent: lower CTE, higher Tg, greater filler loading, stronger initial adhesion, or lower warpage can improve reliability only when the accompanying changes in modulus, relaxation, defects, mode mixity, and aged fracture resistance are also considered. The discussion covers chemical bonding, filler-modified interphases, controlled roughness, and compliant interlayers, with particular attention to the distinction between initial adhesion and long-term durability. Priorities for future work include comparable constitutive and mixed-mode fracture data, long-term hygrothermal aging, and validation of aged coupon or specimen results against full-package lifetime under representative process and service conditions.

Keywords: Advanced Semiconductor Packaging, Polymer Materials, Thermomechanical Reliability, Interface Engineering, Heterogeneous Integration

1. Introduction

Advanced semiconductor packaging sustains gains in integration density and system performance beyond transistor scaling limits [1, 2]. Key technologies such as 2.5D/3D integration, fan-out packaging, and chiplet-based heterogeneous integration rely on polymer dielectrics, epoxy molding compounds (EMCs), and underfills for insulation, protection, mechanical support, and stress redistribution [3-5]. As interconnects shrink and interface density rises, thermal, mechanical, electrical, and moisture effects become increasingly coupled [1, 6]. This intensifies reliability challenges such as warpage, fatigue cracking, and interfacial delamination [6-10]. Packaging reliability hinges on how material formulation and process history jointly govern deformation and local fracture. Prior reviews typically treat polymer dielectrics, EMC warpage modeling, underfill processing, or multi-field reliability as isolated topics [3, 4, 6, 8]. A unified, time-resolved analysis,

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linking formulation, cure, aging, and thermomechanical response to both global warpage and local interfacial fracture, while distinguishing initial adhesion from aged mixed-mode fracture resistance, remains limited.

This review established a unified thermomechanical reliability framework covering warpage, local fracture, and lifetime. It focuses on how polymer properties (CTE, E(T,t), Tg), cure history, package constraints, and moisture drive failure and how interface design modulates that response. Literature is drawn mainly from 2021–2025, supplemented by foundational works on viscoelastic warpage, interfacial fracture, and moisture transport where still essential. Materials covered include PI, PBO, and BCB dielectrics, together with EMCs and underfills; failure modes include warpage, fatigue, delamination, and hygrothermal aging. Emphasis is placed on experimental methods that directly link material state to warpage evolution and crack growth. Electrical properties are addressed only where they constrain polymer or interface design. Solder metallurgy, nonpolymer electrical failures, and device-level mechanisms fall outside this scope. Closing this gap enables consistent interpretation of material trade-offs and objective comparison of interface strategies across materials and architectures. It also identifies the measurements needed to scale coupon-level data to package-specific lifetime predictions—supporting more robust material selection and process design.

2. Polymer materials and property requirements

2.1. Polymer dielectrics

Selecting polymer dielectrics for redistribution layers (RDLs), passivation, and interconnect insulation involves balancing application-specific requirements rather than choosing by material name alone. PI and PBO combine thermal stability, dielectric performance, film-forming capability, and fine-patterning compatibility, whereas BCB offers attractive low-k properties [3]. Formulation and processing remain decisive because CTE, E(T,t), moisture uptake, cure stress, adhesion, and pattern geometry can vary substantially within a nominal material class. The degree of cure and the Cu surface condition can alter residual stress and interfacial fracture resistance even within the same nominal material system. Suitability must therefore be judged in the context of the complete RDL stack and its thermal history.

2.2. Epoxy molding compounds and underfills

Epoxy molding compounds (EMCs) and underfills are both cross-linked polymer systems, but they serve different mechanical functions. EMCs protect the package while their CTE, temperature-dependent modulus, cure shrinkage, thickness, geometry, and molding conditions influence global warpage [4, 8, 11, 12]. Underfills redistribute solder-joint deformation, yet their stiffness and fracture response may shift stress toward die corners or neighboring interfaces [5, 9]. Increasing filler loading can lower CTE and improve heat transport, but it also changes viscosity, wetting, void formation, local stiffness, and fatigue paths [4, 5, 9, 13, 14]. Particle segregation during gap filling may further produce local variations in composition and mechanical properties [15]. Reducing global deformation is beneficial only when it does not redistribute or localize strain onto a weaker failure path.

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2.3. Coupled property trade-offs

Packaging polymers must satisfy coupled electrical, thermal, mechanical, environmental, and processing constraints. Lower CTE and a suitable modulus can limit structural deformation, while Tg should be selected relative to the cure, reflow, thermal-cycling, and service-temperature windows [3, 8]. Fine-pitch interconnects also require low dielectric loss, low moisture uptake, reliable metallization adhesion, and practical manufacturability. High-power packaging imposes more stringent thermal-conductivity requirements [3, 14]. Heavy filler loading can raise thermal conductivity and lower CTE, but may also increase dielectric loss, viscosity, interfacial defects, and local stiffness mismatch [5, 14, 16]. Molecularly engineered heat-conduction pathways may reduce reliance on high filler loading, however, their practical applicability still requires validation of cure behavior, adhesion, moisture response, and performance in mechanically constrained multilayer stacks [16]. Property specifications should identify the formulation, process history, temperature window, package constraint, and test method under which a value was obtained. Reported values are formulation- and test-dependent, not intrinsic constants of a broad material class (Table 1).

Table 1. Representative polymer classes in advanced packaging [3-5, 8, 9, 14]

Material	Typical role	Key Strengths / Trade-offs	Main reliability concerns
PI	RDL dielectric / insulation	Thermal stability, mature processing, Moisture and CTE are formulation-dependent	Cu/PI delamination, RDL stress / cracking
PBO	RDL dielectric / passivation	Dielectric and patterning performance, Process compatibility is critical	Passivation/RDL cracking, interface failure
BCB	Low-k RDL dielectric	Low dielectric constant, Mechanical robustness and adhesion can constrain integration	Stress localization, metal/dielectric adhesion loss
EMC	Encapsulation	Tunable CTE, stiffness, and thermal transport through fillers	Warpage, corner stress, moisture-assisted delamination
Underfill	Flip-chip redistribution	Reduces solder-joint strain, performance depends strongly on cue and filler morphology	Thermal-fatigue cracking, die-corner/interfacial damage

3. Thermomechanical reliability and failure mechanisms

Thermomechanical reliability is governed by the competition between the package-level crack-driving force, G, and the evolving interfacial fracture resistance, Gc. Neither warpage magnitude nor initial adhesion strength alone is sufficient to predict lifetime [17-21]. Material and process variables establish mismatch strain, stress evolution, and the local balance between G and Gc, these state variables then govern global warpage, crack initiation and growth, and ultimately package-specific lifetime. The framework emphasizes that a lower global response does not necessarily reduce the local crack-driving force, so warpage should be interpreted together with G, Gc, mode mixity, crack path, and fatigue behavior (See Figure 1).

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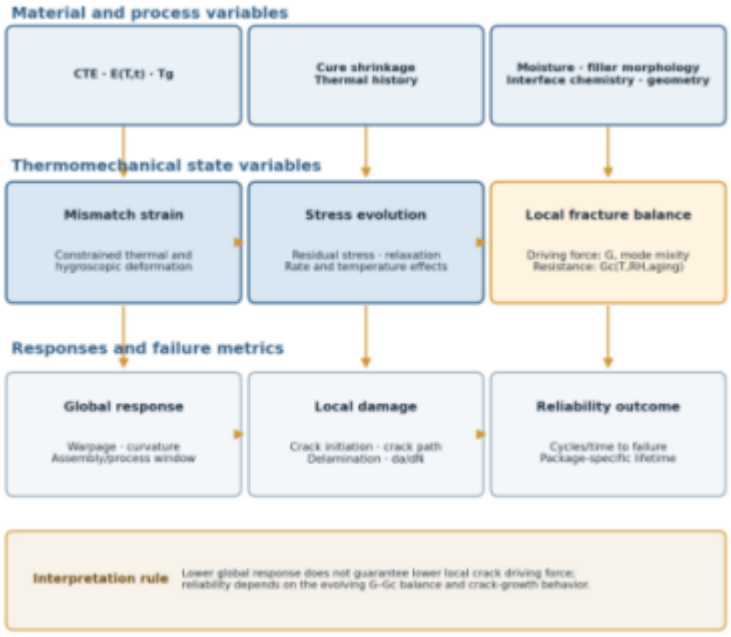

Figure 1. Schematic framework linking polymer and processing variables to thermomechanical state evolution, global package response, local fracture, and reliability outcomes [6, 9-11, 17, 20, 22]

3.1. CTE mismatch and viscoelastic stress evolution

Heterogeneous integration combines silicon, copper, solder, polymer dielectrics, underfills, and EMCs within constrained multilayer architectures. Differences in constituent CTE generate incompatible free strains during cure, reflow, thermal cycling, and device operation. These structural constraints convert free-strain mismatch into stress and produce stress concentrations at structural discontinuities, die corners, free edges, and RDL transition regions [6].

Polymer stresses are strongly time- and temperature-dependent. The polymer modulus changes substantially near Tg, while viscoelastic relaxation redistributes stresses generated during cure and thermal excursions over the relevant dwell-time scale [11]. Package response consequently depends on CTE together with E(T,t), Tg, cure shrinkage, thickness, geometry, process conditions, and thermal history [8, 11, 12]. A Tg above the service window can preserve dimensional stability, but it may also retain glassy stiffness and residual stress. When Tg lies within the cycling window, the package experiences a large stiffness change, a lower Tg allows more relaxation but may reduce structural support. The ratio of the material relaxation time to the process or cycle dwell time governs how much stress remains at each stage. Thus, the same CTE mismatch can produce different stress fields below, across, and above Tg, or after different cure dwells. Fan-out studies likewise show that EMC CTE and modulus must be interpreted within the complete stack [12]. These coupled effects determine not only global package deformation but also the local crack-driving conditions discussed below.

3.2. Warpage and thermal fatigue

The through-thickness distributions of mismatch strain and stiffness govern package curvature and warpage. Viscoelastic and process-based studies show that warpage depends on temperature-

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dependent material behavior, encapsulation and cure conditions, geometry, and interlayer configuration rather than on CTE alone [8, 11, 12]. Excessive warpage can compromise handling, alignment, interconnection, and assembly, bending and corner constraints may also amplify local stress [6, 12]. Lowering EMC CTE is most beneficial when global mismatch curvature dominates and the effects of modulus, cure shrinkage, flow behavior, and defects remain comparable. If the CTE reduction is achieved through stiffening or heavy filler loading, global curvature may fall while the local interfacial crack-driving force rises. Warpage measurements are therefore most informative when paired with local stress or G at a critical interface and with evidence of the crack path. A flatter package is not necessarily less vulnerable to local failure.

Repeated temperature excursions convert the evolving stress field into fatigue damage. Silica-filled underfills have shown thermal-fatigue crack initiation and propagation at lower fracture-mechanics driving forces than conventional mechanical fatigue tests, with filler content altering crack initiation, path, and growth resistance [9]. Filler-induced CTE reduction and stiffness may reduce overall deformation while the particle–matrix microstructure creates debonding, deflection, or stress-concentration pathways.

3.3. Interfacial delamination

Interfacial delamination is a local outcome of this thermomechanical sequence. Pre-existing edge defects or weak interfacial regions provide likely crack-initiation sites [7, 18, 19, 23]. Stress concentrations near free edges, corners, polymer/metal boundaries, polymer/silicon interfaces, and multilayer films can activate these sites [6, 7, 18, 19, 23]. Subsequent thermal excursions extend the crack as the surrounding materials expand, contract, and relax. Nominal adhesion strength alone is an insufficient reliability metric because it does not capture crack geometry, mixed-mode loading, roughness-dependent crack paths, or crack-growth resistance [17-19, 23].

Fracture mechanics distinguishes the crack-driving force, characterized by the energy release rate G and mode mixity, from the interfacial fracture resistance Gc [17-19]. Delamination develops as the local driving force approaches the relevant resistance, and both evolve with temperature, loading history, crack path, and environment [7, 10, 17-19]. Package geometry, residual stress, loading, and defect size determine G, whereas measured Gc depends on mode mixity and on whether the crack remains at the interface or enters a neighboring layer. Interpreting apparent fracture toughness therefore requires observation of the crack location and propagation path. Surface treatment may raise initial peel strength without improving thermal-cycling resistance, while geometry or residual stress can destabilize an interface that appears strong in a coupon test. Quantitative assessment of PI-RDL delamination under accelerated stress further underscores the need for package-relevant validation rather than reliance on a single adhesion metric [22].

3.4. Hygrothermal degradation

Moisture can alter both the interfacial crack-driving conditions and the interfacial fracture resistance. Moisture uptake induces hygroscopic swelling and may alter the polymer modulus, Tg, and interfacial chemistry. Transport is itself dependent on temperature and exposure history, so diffusion models based only on constant material parameters have limited value under dynamic thermal loading [24, 25]. Rapid heating of a conditioned package can combine hygroscopic deformation, thermal mismatch, and moisture-related stresses, increasing the driving force for separation. Coupled package models show that concentration history, temperature, and fracture behavior jointly determine moisture-induced delamination [20, 26].

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Temperature and moisture uptake can reduce mixed-mode fracture toughness at EMC/printed-circuit-board and polymer/metal interfaces [10, 21]. Hygrothermal reliability is therefore history-dependent: exposure changes the moisture field, constitutive response, residual stress, interface chemistry, and Gc. The state at fracture loading is set by conditioning time, diffusion length, desorption during reflow, and the temperature dependence of transport. Treating thermal, mechanical, and moisture effects as separate additive loads overlooks their combined tendency to increase the driving force while reducing interfacial fracture resistance [6, 10, 20, 21, 26].

3.5. Conditional design rules for reliability

Table 2. Conditional design rules and limitations of common single-property assumptions

Design rule	Valid when	Failure mode / limitation	Better interpretation
Lower CTE	Global mismatch deformation dominates	Stiffness / filler may raise local stress	Evaluate CTE with E(T,t), geometry, G and Gc
Higher Tg	Service/reflow range remains below Tg	High glassy stiffness and cure stress may increase loading	Select Tg relative to cure, reflow, cycling, and service windows
Higher filler loading	Dispersion, wetting, and cure remain controlled	Viscosity, voiding, stiffness gradients, fatigue paths	Optimize loading with morphology, interphase, and processability
Higher initial adhesion	Interface chemistry remains stable	Aging may reduce Gc, crack path may change	Separate initial adhesion from aged mixed-mode fracture resistance
Rougher Cu	Roughness improves anchoring without harming wetting / integration	Excess roughness can create defects and stress nonuniformity	Optimize roughness scale and chemistry, not maximum Ra
Lower warpage	Global deformation dominates failure	Local G may increase despite flatter package	Pair warpage with local G, Gc, crack path, and fatigue

Table 2 summarizes the conditions under which CTE, Tg, filler loading, adhesion, Cu roughness, and warpage affect lifetime, as well as the main reasons that single-property rules fail [8-11, 13, 14, 22, 23, 27, 28] .

4. Interface engineering, durability, and future directions

Based on the failure mechanisms discussed in Section 3, interface engineering should be viewed as the coordinated control of bonding chemistry, local stiffness, crack-path geometry, and long-term fracture resistance. Interface treatments alter either bonding chemistry or the way load is transferred across the joint. Their value depends on the crack path, thermal history, and integration constraints, and gains in initial adhesion should be separated from changes in long-term durability.

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4.1. Chemical bonding and surface activation

Chemical approaches strengthen weak interfaces by controlling polymer functional groups, adhesion promoters, surface energy, and metal-oxide chemistry. Studies of smooth Cu surfaces and Cu RDLs—including oxide control, silane coupling, molecular interactions, and plasma activation—show the importance of surface chemistry to interfacial behavior [29-31]. These approaches can enhance interfacial bonding without the electrical and geometrical penalties associated with aggressive surface roughening. The reported results clarify initial bonding mechanisms, longer-term performance depends on how surface chemistry and residual stress evolve after bonding.

Surface activation may decay before bonding, adhesion promoters respond to cure history, and oxide/polymer interfaces continue to evolve under heat and moisture. Relevant measurements therefore include surface chemistry before bonding and after aging, aged mixed-mode fracture resistance, and response in the intended geometry [10, 21, 32]. Useful comparative descriptors include oxide thickness, functional-group density, and water contact angle. These should be measured after fracture specimens have undergone the same reflow and environmental conditioning history.

4.2. Filler and interphase engineering

Filler and interphase engineering affect both bulk material properties and local load transfer. Functionalized silica can improve dispersion, wettability, rheology, and stress transfer at the particle–matrix boundary [13]. Strong particle–matrix bonding suppresses agglomeration and debonding. By contrast, overly stiff local regions or weakly bonded particle–matrix interfaces may become preferential crack-initiation sites. The response depends on particle size and shape, surface treatment, loading, cure route, viscosity, sedimentation, and flow. For a given formulation, bulk CTE, modulus, and fatigue data are best interpreted alongside fractography and dispersion measurements.

4.3. Controlled mechanical interlocking

Controlled surface microtopography can promote mechanical interlocking and delay debonding or interfacial crack initiation. Results for nodulated Cu and laminated epoxy composite films show that as-bonded adhesion is sensitive to surface morphology [27, 28], while fracture studies demonstrate that roughness can redirect crack paths [23]. Interlocking is most effective when the polymer fully wets the surface features and their characteristic scale forces a longer crack path or a mixed cohesive–interfacial path. Excessive roughness, however, may compromise fine-line patterning, high-frequency performance, wetting behavior, and stress uniformity. It may also trap voids and offset the gain in apparent adhesion.

A meaningful description of roughness extends beyond Ra to include feature wavelength and shape, oxide chemistry, polymer wetting, and penetration into the surface profile. By coordinating these variables with lamination and cure conditions, effective mechanical interlocking can be achieved while maintaining fine-line integration capability. For high-frequency lines, the allowable roughness must also satisfy conductor-loss and patterning constraints.

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4.4. Gradient and compliant interfaces: emerging opportunities and limitations

Graded or compliant interphases distribute load over a finite thickness, smoothing an abrupt modulus change while retaining enough constraint for dimensional stability. Current support comes mainly from neighboring composite research [33], in which interphase dimensions and processing differ from those in fine-pitch packaging. In practical packaging applications, graded or compliant interphases require precise control of interlayer thickness, compatibility with cure and reflow processes, dielectric performance, adhesion, and hygrothermal stability. An overly thick layer may add excessive compliance, whereas a very thin layer may redistribute little stress. For now, the concept is best regarded as a testable packaging hypothesis rather than an established solution.

4.5. Long-term interface durability and validation

During elevated-temperature aging, epoxy/Cu interfaces can undergo Cu diffusion and environmentally induced or catalyzed polymer degradation [32]. Temperature and moisture also affect transport, chemistry, mixed-mode toughness, and the balance between G and Gc [10, 20, 24, 25]. Durability datasets are most useful when they report surface preparation, cure history, specimen geometry, mode mixity, loading rate, temperature, humidity, E(T,t), crack path, fracture resistance, and specimen-to-specimen variation. Combining these measurements allows degradation of the material state or interfacial fracture resistance to be distinguished from increases in the external crack-driving force.

Based on the literature reviewed, a four-level validation sequence can be proposed: as-bonded chemistry and coupon adhesion, aged mixed-mode fracture under controlled temperature and moisture, constitutive and crack-growth verification in a representative subcomponent, and full-package validation of warpage, delamination, and lifetime under realistic cure, reflow, cycling, and hygrothermal histories [17, 18, 20-22]. Parameters carried between levels must retain their dependence on temperature, loading rate, fracture-mode mixity, and aging state. The most pressing measurements are long-term aging curves, E(T,t), mixed-mode crack-growth resistance, and observations of buried crack paths under package-relevant thermal and moisture histories.

The same constitutive, hygrothermal, fracture, and lifetime measurements could also provide a practical basis for evaluating self-healing polymers and data-driven models [34, 35].

5. Conclusion

Thermomechanical reliability arises from the interaction among material formulation, process history, package constraints, and interfacial fracture. CTE mismatch generates incompatible strains, while E(T,t), Tg, cure shrinkage, geometry, filler morphology, and moisture determine whether these strains relax, drive global package curvature, or localize near critical interfaces and cracks. Warpage and local fracture therefore provide complementary reliability metrics: package curvature characterizes the global structural response, whereas G, Gc, crack path, and fatigue crack-growth behavior govern local delamination. Moisture introduces additional coupling because it can simultaneously increase the crack-driving force and reduce the interfacial fracture resistance.

Material-selection rules are useful only when their applicable conditions are stated. Lowering CTE improves reliability when mismatch curvature dominates and the accompanying stiffness or defects do not transfer load to a critical interface. Tg should be selected relative to the cure, reflow, thermal-cycling, and service-temperature windows. Filler content must be assessed together with dispersion, rheology, void formation, and fatigue behavior. Chemical bonding and controlled surface

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topography can strengthen an interface, while compliant or graded interphases may redistribute stress. Their benefit nevertheless depends on the local crack path, the chemical state of the aged interface, and the constraints imposed by the intended integration process.

Further progress requires measurements that connect material state to package failure across the four validation levels: as-bonded chemistry and coupon adhesion, aged mixed-mode fracture, representative subcomponents, and full-package lifetime. Particularly valuable data include E(T,t), temperature- and moisture-dependent Gc, mode mixity, crack-growth rate, observations of buried interfaces, and complete cure and aging histories. Such data would give material formulation and interface design a common physical basis. They would also allow emerging self-healing polymers and data-driven reliability models to be assessed under representative manufacturing and service histories.

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