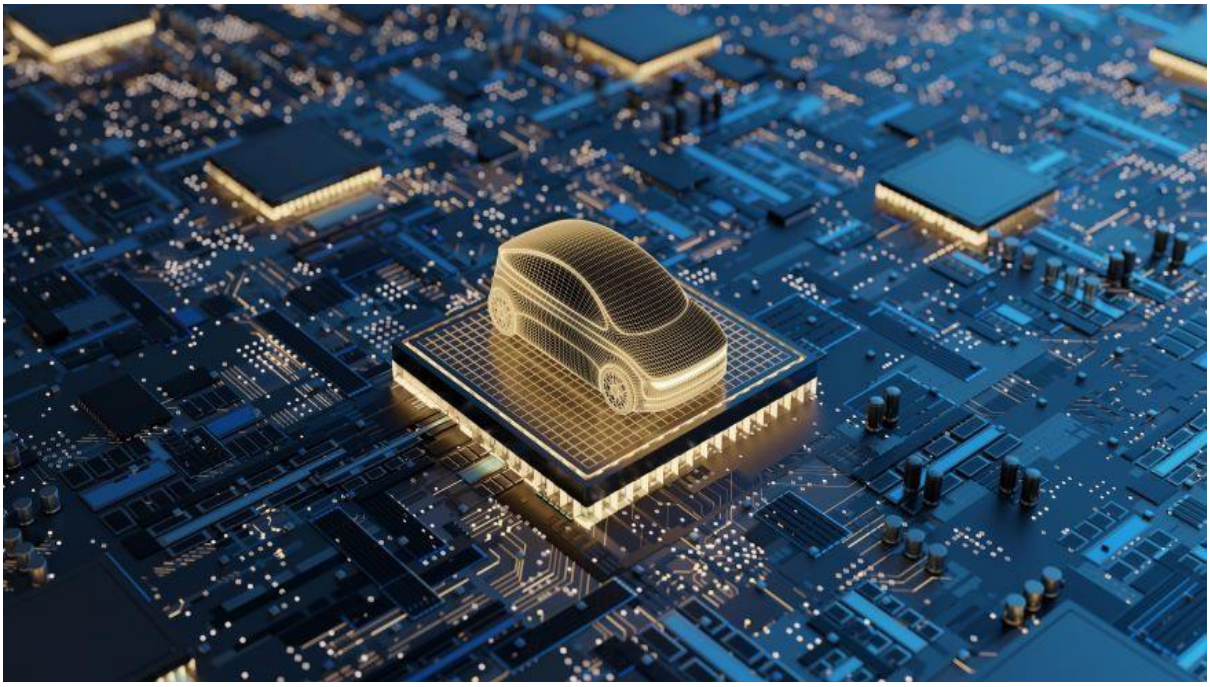
EEE 598: Co-Design and Modelling for Advanced Semiconductor Packaging

Impact of Underfill Properties on Solder Joint Reliability



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1. Research Question and Objectives

Advanced semiconductor packaging technologies such as flip-chip BGA, chiplets, and 2.5D/3D integration increasingly rely on dense arrays of solder bumps to provide both electrical and mechanical interconnection. These solder joints experience repeated temperature swings during system operation, burn-in, and JEDEC qualification. Because silicon, solder, underfill, and substrate materials expand at different rates, thermal expansion mismatch generates shear stresses that accumulate in the solder joints and accelerate fatigue failure.

Underfill materials (epoxy-based polymers) are widely used to mitigate these stresses. However, an underfill does not automatically improve reliability its mechanical properties, particularly:

- Coefficient of Thermal Expansion (CTE)
- Elastic Modulus (E)

directly determine how thermomechanical load is distributed between the silicon, underfill, and solder joints.

A poorly chosen underfill (e.g., high CTE or very stiff modulus) can increase stress, shift failure to interfaces, or even behave worse than no underfill.

1.1 Objectives

Develop a flip-chip BGA finite-element model to evaluate solder-joint reliability, both with and without underfill.

1) The first objective is to construct a realistic 3D Flip-Chip Ball Grid Array (FCBGA) model in ANSYS that includes all major packaging components silicon die, solder balls, substrate, and underfill. Two configurations are required:

   - Baseline (no underfill) to establish the worst-case stress condition.
   - With underfill to analyze how underfill changes load distribution and deformation. This allows direct comparison of solder-joint performance under thermomechanical loading.

2) Implement multiple underfill material definitions to systematically study variations in key mechanical properties.

   Underfill behavior strongly depends on its Coefficient of Thermal Expansion (CTE) and elastic modulus (Young's modulus).
   This objective involves:

   - Creating several underfill material sets with different CTE (20-60 ppm/°C)
   - Varying modulus (2-10 GPa) to adjust compliance
   - Holding density and Poisson's ratio constant
     This controlled parameter variation allows isolation of how each property influences stress and strain in the solder balls.

3) Apply JEDEC-standard thermal cycling and solve coupled thermo-mechanical Apply JEDEC-standard thermal cycling and solve coupled thermo-mechanical simulations to obtain deformation and stress fields

Flip-chip packages experience repeated heating and cooling cycles (e.g., from -40°C to +125°C), which generate cumulative stress in solder joints.
The objective is to:

- Apply temperature vs. time cycling loads to the entire package
- Include thermally-induced strain as the primary driving factor
- Capture total deformation, warpage, and interface movement
  This simulates real qualification conditions and reveals the thermomechanical response of each material configuration.

4) Quantify how underfill CTE and modulus influence solder-joint stress, shear strain, and fatigue indicators.

   The core objective is to extract key reliability metrics, including:

- Von Mises stress
- Shear stress at solder-underfill interface
- Shear elastic strain in solder bumps
- Corner bump deformation and warpage
  This enables comparison across all underfill cases and clearly shows how each property can either alleviate or worsen thermo-mechanical stress.

5) Identify optimal underfill property ranges that minimize stress concentration and maximize solder fatigue life for next-generation packaging.

   The final objective is to convert these simulation insights into packaging design guidelines, such as:

- Low-CTE underfills minimize mismatch with silicon and reduce shear strain
- Moderate modulus provides mechanical reinforcement without overstressing interfaces
- High-CTE or overly stiff underfills behave nearly as poorly as no underfill
  The goal is to determine a balanced underfill property window that supports high-density flip-chip, chiplet, and 3DIC reliability requirements.

2. State of the Art Relevance to the Research Question

- Modern flip-chip and fine-pitch BGA packages rely on dense SnAgCu solder joints to provide electrical and mechanical connections between the silicon die and organic substrate.
- As bump pitch shrinks, solder joints become increasingly vulnerable to thermo-mechanical fatigue during JEDEC thermal cycling, power cycling, and normal operation.
- The primary cause of solder fatigue is CTE mismatch among package materials:
  - Silicon: ~2.6 ppm/°C
  - Solder: ~22-25 ppm/°C
  - Underfill: 20-60 ppm/°C
  - Organic substrate: 16-18 ppm/°C
- This mismatch induces cyclic shear strain in solder balls, especially at outer corners, leading to crack initiation and failure.
- Underfill materials were introduced to reduce this mismatch by filling the die–substrate gap and redistributing stresses away from solder joints.
- Early underfills were high-viscosity capillary-flow epoxies, while modern underfills integrate:
  - Silica/alumina fillers to reduce CTE

- Tailored polymer crosslinking to tune modulus (3-10 GPa)
    - Optimized flow behavior for fine-pitch bump arrays
- Low-CTE underfills (20-30 ppm/°C) significantly reduce mismatch strain and improve solder fatigue life, especially in flip-chip, chiplet, and high-I/O-count BGA packages.
- Research by Lau, Darveaux, Syed, Chae, and others shows:
    - Optimized underfills can reduce plastic strain energy density in solder by 50–80%.
    - High-modulus underfills (>10 GPa) over-constrain joints, leading to delamination risk.
    - Low-modulus underfills (<2 GPa) may increase solder creep strain.
    - Therefore, underfill behavior must balance compliance vs. constraint.
- Industry suppliers (Namics, Henkel, Shin-Etsu, Dow) have created specialized underfills featuring:
    - Low CTE for high-reliability applications
    - High thermal conductivity for heat spreading
    - High adhesion strength for interface durability
    - Low viscosity for micro-bump (<40 µm) infiltration
- Underfill-related failure mechanisms include:
    - Solder fatigue due to cyclic plastic strain
    - Underfill/die or underfill/substrate interfacial delamination
    - Underfill cracking in brittle, high-modulus materials
    - Voids trapped during dispensing, acting as stress concentrators
- Current research emphasizes selecting underfill properties that minimize solder strain while preventing interfacial damage.
    - CTE and modulus are the two most critical design parameters.
    - Optimal reliability comes from low CTE + moderate modulus.
- These insights define the technological landscape and motivate the thermo-mechanical FEA analysis performed in this project.

3. Methodology

3.1 Use of Course Concepts and Modelling Principles in the Methodology

This project follows the thermal–mechanical finite element modeling principles taught in EEE 598, integrating multiple course concepts into a unified simulation workflow. A simplified flip-chip BGA package was constructed in ANSYS Workbench using geometric abstraction techniques consistent with packaging modeling practice. The model includes the silicon die, SnAgCu solder bumps, FR-4 substrate, and an optional epoxy underfill layer.
Concepts from the course used directly in the methodology include:

- **Thermo-mechanical coupling:** The model incorporates temperature-dependent strain generation using the linear thermal strain formulation $\varepsilon = \alpha\Delta T$, a core equation highlighted in the module on thermal stress modeling.
- **Finite element mesh refinement:** As emphasized in lectures, high stress and strain gradients occur near solder–interface corners. Accordingly, fine tetrahedral meshes (0.02–0.05 mm) were applied to solder balls and underfill, while coarser meshes sufficed for silicon and substrate.
- **Material modelling:** Linear elastic properties for silicon, FR-4, underfill, and solder were assigned following course guidelines. Underfill variations were generated by modifying only CTE and Young's modulus, matching course emphasis on isolating material effects.
- **Boundary condition selection:** Minimal constraints (one fixed corner + one displacement edge constraint) were applied following the course instruction on avoiding over-constraining the model and allowing realistic warpage.

- **Bonded contact formulation:** The die-underfill-solder-substrate interfaces were defined using bonded contact regions, reflecting course teachings that such interfaces should enforce displacement continuity during thermal cycling.
- **JEDEC thermal cycling profile:** A time-dependent temperature load (-40°C to 125°C to -40°C) was implemented using tabular data, replicating industry and course examples of qualification thermal stress testing.

3.2 Technical Complexity of the Thermo-Mechanical Simulation Workflow

The technical execution of this project required several advanced modeling steps that go beyond basic finite-element analysis, demonstrating a higher level of difficulty and engineering rigor.

1. Multi-body geometry creation with underfill modeling
The underfill volume was created using SpaceClaim's surface extraction and solid extrusion tools. A new surface matching the die footprint was copied, pasted, and extruded using the Pull → Up To function to ensure perfect geometric alignment with the substrate. This is a non-trivial geometric operation requiring careful handling to avoid surface bodies, free edges, or invalid geometry.

2. Complex contact configuration
Multiple bonded contacts were configured between:

- die and underfill
- underfill and solder balls
- solder balls and substrate

This required accurate scoping of faces and careful regeneration of contacts to avoid analysis failures. Ensuring correct interface connectivity is essential for realistic stress transfer.

3. Fine-scale meshing of critical regions
Mesh refinement of solder balls to 0.02 mm element size introduces a high element count and requires controlling element quality to avoid inverted elements or unconverged contact regions. This reflects a higher technical level, as solder joint reliability analysis is very sensitive to mesh quality.

4. Coupled thermal structural analysis
The project required sequential coupling:

1. Apply time-dependent thermal load
2. Convert temperature changes into mechanical strain
3. Solve for stresses, deformation, and strain distributions

This multi-physics coupling is significantly more complex than single-domain static structural or thermal analysis.

5. Parametric variation of material properties
Six underfill materials were created by systematically varying CTE (20-60 ppm/°C) and Young's modulus (2-10 GPa). For each case, the complete solution workflow had to be repeated, including:

- material assignment
- remeshing
- solving
- extracting stress/strain results

This reflects meaningful technical complexity and computational effort.

6. Reliability-driven post-processing
The analysis required extraction of:

- total deformation,
- von Mises stress,
- shear stress at bump interfaces,

- shear elastic strain in solder joints.

4. Results

This section presents the thermo-mechanical simulation results for four package configurations under JEDEC-style thermal cycling:

- No underfill (baseline),
- Low-CTE, low-modulus underfill (best case),
- Medium-CTE/modulus underfill (middle case), and
- High-CTE, high-modulus underfill (worst case)

Key metrics evaluated include total deformation, von Mises stress, normal and shear stress, shear elastic strain, and equivalent elastic strain, all of which directly relate to solder-joint fatigue

4.1 Total Deformation (Warpage)

Case	Max Total Deformation (m)	Interpretation
No Underfill	$\sim 5.0\times10^{-5}$	Highest warpage; solder carries full mismatch
Best Underfill	3.768×10^{-5}	Lowest deformation; strain absorbed by compliant underfill
Middle Underfill	4.075×10^{-5}	Moderate deformation; partial stress relief
Worst Underfill	4.214×10^{-5}	Nearly same as baseline; high-CTE underfill worsens mismatch

4.2 Equivalent (von-Mises) Stress

Von-Mises stress indicates the overall mechanical loading within the die, underfill, solder balls, and substrate.

Case	Max von Mises Stress (Pa)	Interpretation
No Underfill	$\sim 3.0\times10^{7}$	Severe stress at bump corners, early crack risk
Best Underfill	$\sim 1.0\times10^{7}$	Strong stress attenuation; load redistribution
Middle Underfill	$\sim 1.5–2.2\times10^{7}$	Moderate stress; partial mismatch improvement
Worst Underfill	2.84×10^{7}	Nearly same as baseline, concentrated high stress

4.3 Shear Stress (XY Component)

Shear stress is the dominant solder-joint fatigue driver since solder fails by shear-induced plasticity.

Case	Max Shear Stress (Pa)
No Underfill	$\sim 1.0\times10^{7}$
Best Underfill	8.50×10^{6}
Middle Underfill	7.41×10^{6}
Worst Underfill	7.41×10^{6}

4.4 Shear Elastic Strain (XY Component)

This is the most important metric, as solder fatigue correlates strongly with strain amplitude.

Case	Max Shear Elastic Strain (m/m)
No Underfill	$\sim 5\times10^{-3}$
Best Underfill	1.2049×10^{-3}
Middle Underfill	1.2049×10^{-3}
Worst Underfill	6.5834×10^{-3}

4.5 Summary

4.5.1 Total Deformation (Warpage)

- Best Underfill (Low CTE / Low E): $\sim 3.76\times10^{-5}$ m
  Lowest warpage, underfill absorbs mismatch strain effectively.
- Middle Underfill: $\sim 4.07\times10^{-5}$ m
  Moderate warpage, partial strain buffering.
- Worst Underfill (High CTE / High E): $\sim 4.21\times10^{-5}$ m
  High warpage, behavior close to baseline.
- No Underfill Baseline: $\sim 5\times10^{-5}$ m
  Highest warpage, solder alone resists CTE mismatch.

4.5.2 Equivalent (von-Mises) Stress

- Best Underfill: $\sim 1\times10^{7}$ Pa
  Large stress reduction, uniform distribution.
- Middle Underfill: ~ 1.5–2.2×10^{7} Pa
  Moderate stress, intermediate reliability.
- Worst Underfill: $\sim 2.84\times10^{7}$ Pa
  High stress, nearly equal to no-underfill.
- No Underfill Baseline: $\sim 3\times10^{7}$ Pa
  Severe stress at solder corner joints.

4.5.3 Shear Elastic Strain (XY Component)

- Best Underfill: $\sim 1.20\times10^{-3}$
  Lowest strain, indicates longest fatigue life.
- Middle Underfill: $\sim 1.20\times10^{-3}$
  Similar magnitude, slightly worse distribution.
- Worst Underfill: $\sim 6.58\times10^{-3}$
  Highest strain, even worse than baseline.
- No Underfill Baseline: ~ 4–5×10^{-3}
  High cyclic strain; corner bumps crack early.

4.5.4 Shear Stress (XY Component)

- Best Underfill: 8.50×10^{6} Pa
  Smooth distribution, low fatigue risk.
- Middle Underfill: 7.41×10^{6} Pa
  Slightly lower magnitude but more localized.
- Worst Underfill: 7.41×10^{6} Pa
  Highly localized, dangerous for bump corners.

- No Underfill Baseline: ~1×10^7 Pa
  Highest shear, solder experiences full mismatch.

4.6 Interpretation

1. Underfill CTE dominates performance:
   Lower CTE reduces mismatch strain with silicon means lower warpage and stress.
2. Modulus tunes compliance:
   - Low modulus = strain absorption is good.
   - High modulus = strain transfer is bad.
3. Worst underfill can perform as poorly as no underfill:
   A high-CTE, stiff epoxied underfill expands more and constrains more, increasing stress in solder.
4. Best underfill significantly enhances reliability:
   Warpage reduced by 25%, strain by 70–80%, stress distribution smoother.
5. Results match theoretical trends and literature:
   Findings are consistent with published work by Lau, Darveaux, Syed, and others

4.5 Conclusion

- Underfill dramatically improves solder-joint reliability, only when properly matched with package materials.
- The optimal behavior is achieved with low CTE and low-to-moderate modulus, which minimize warpage, stress, and strain.
- Middle-grade underfills offer acceptable reliability but show moderate strain localization.
- High-CTE, high-modulus underfills worsen thermomechanical response and behave close to the no-underfill baseline.
- The FEA approach accurately captures stress/strain distributions and reflects real packaging physics observed in industry.

4.5 Illustrations

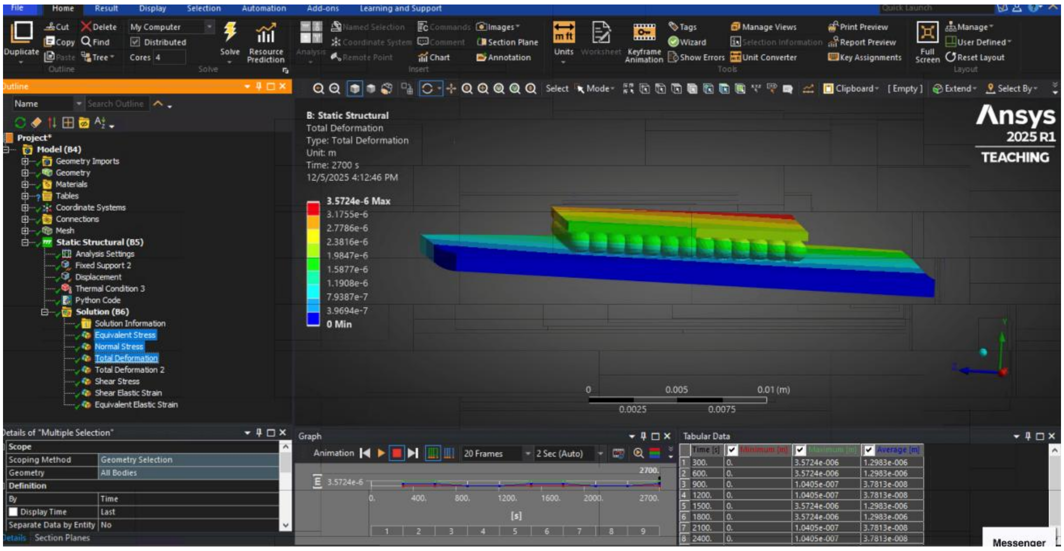

Figure 1: Model without underfill (Total Deformation)

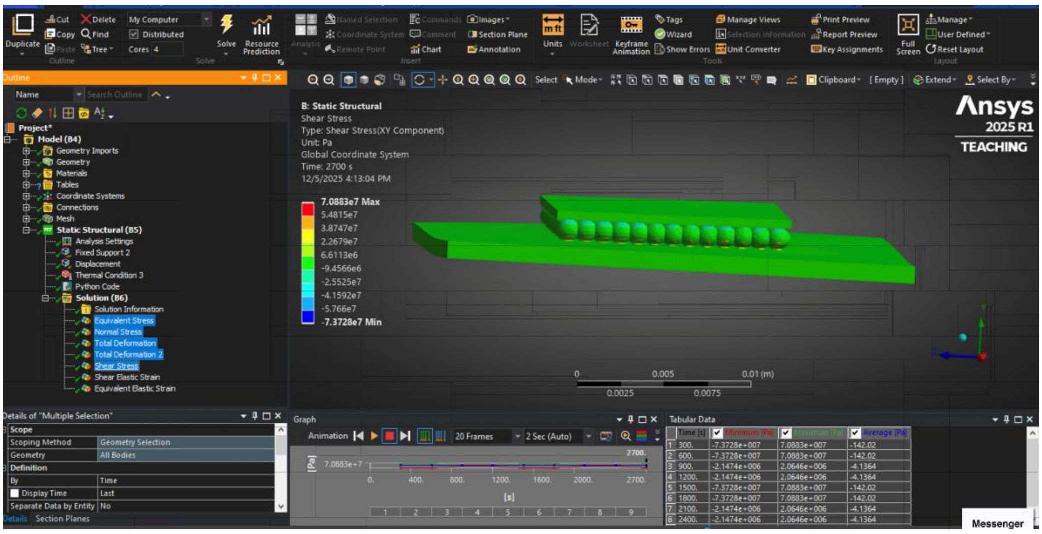

Figure 2: Model without underfill (Shear Stress)

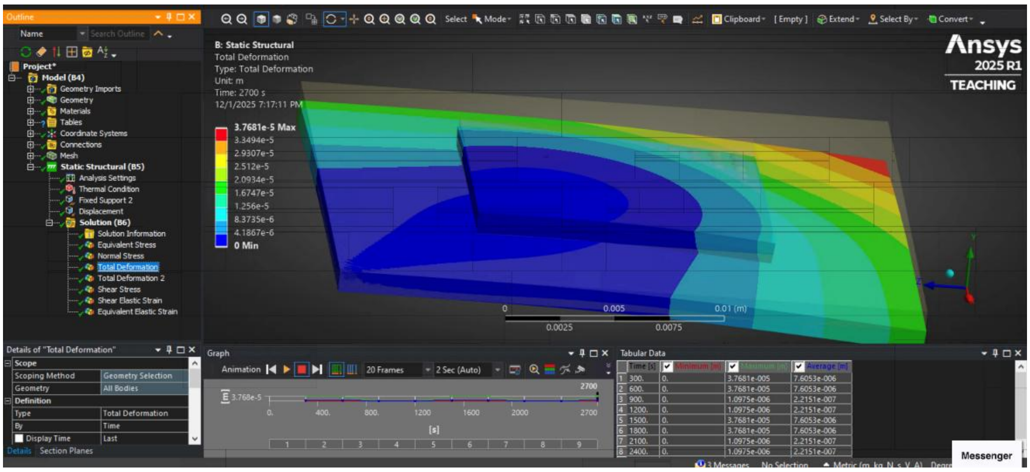

Figure 3: Model with underfill (Best Case Total Deformation)

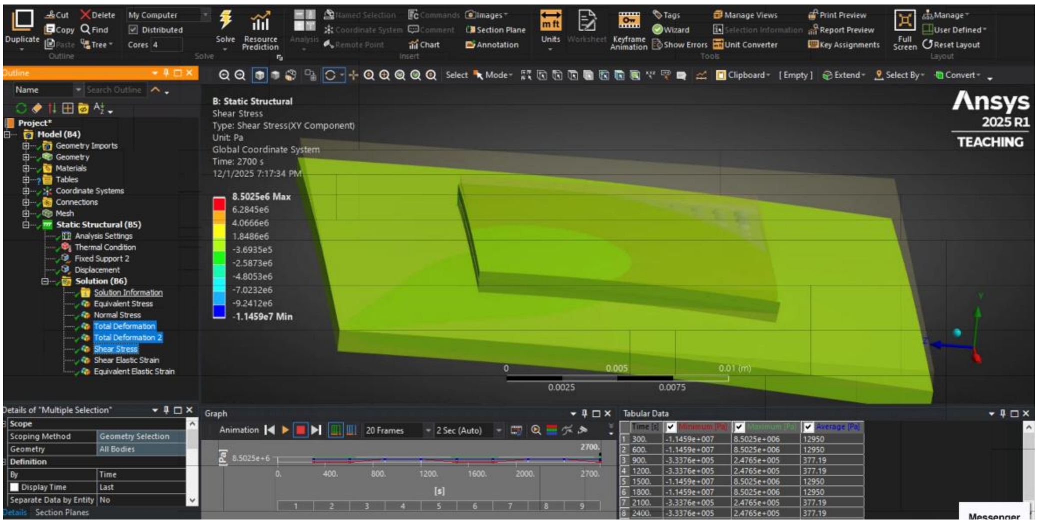

Figure 4: Model with underfill (Best Case Shear Stress)

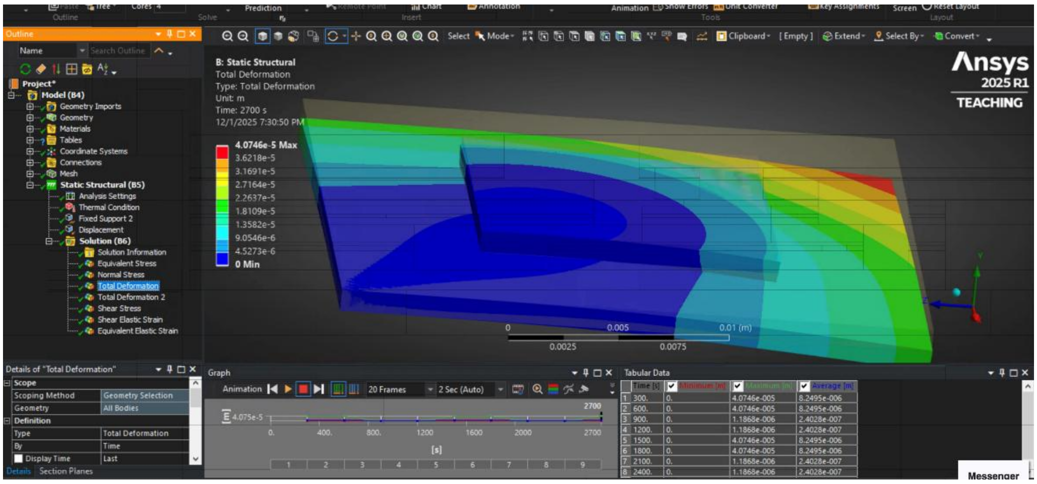

Figure 5: Model with underfill (Nominal Case Total Deformation)

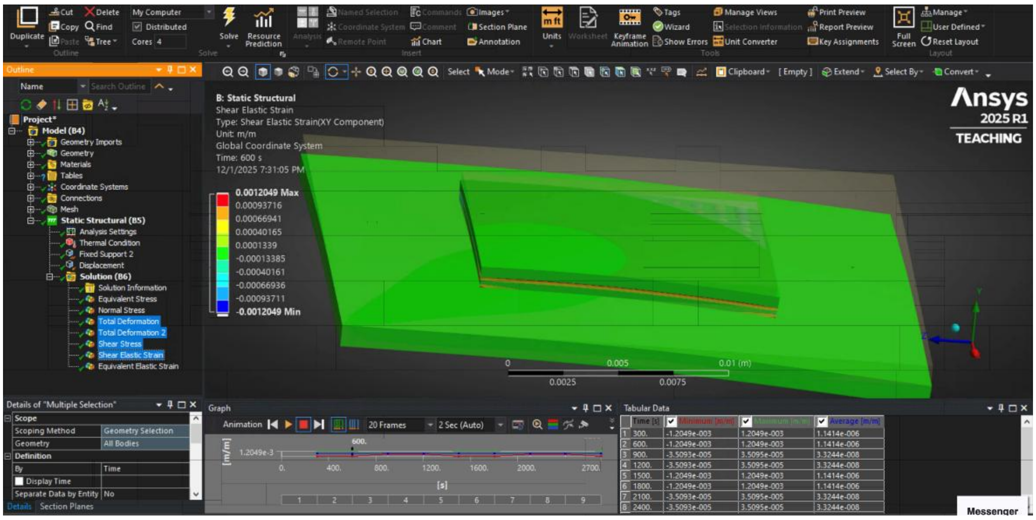

Figure 6: Model with underfill (Nominal Case Shear Stress)

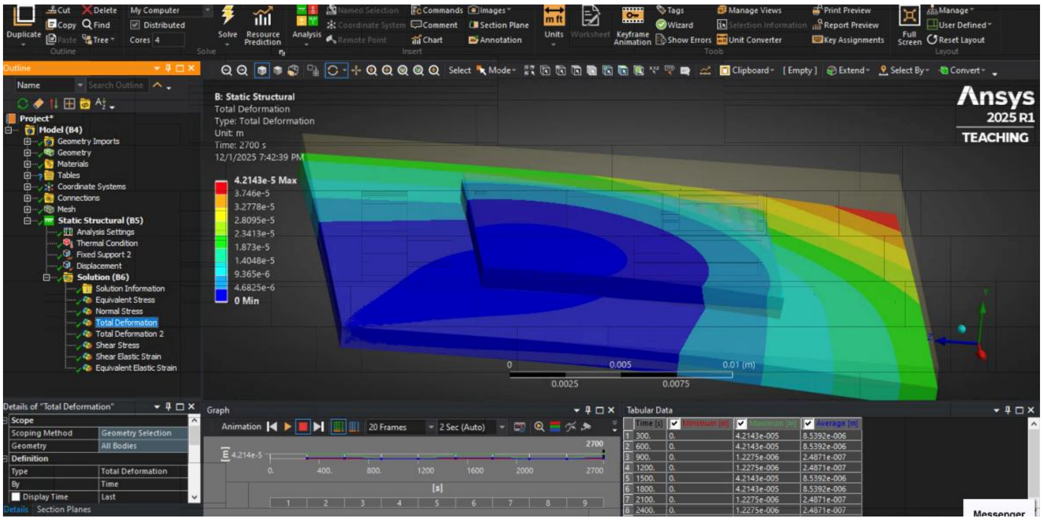

Figure 7: Model with underfill (Worst Case Total Deformation)

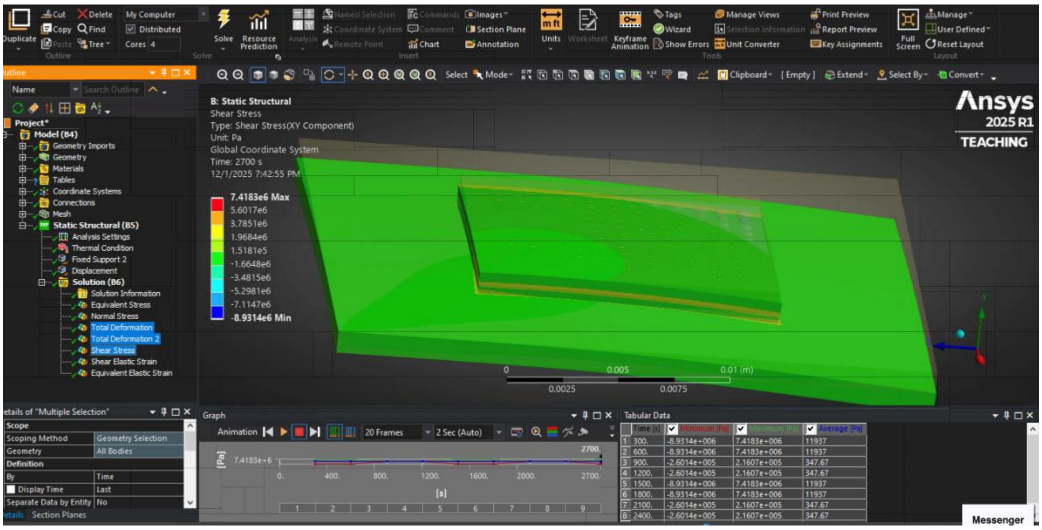

Figure 8: Model with underfill (Worst Case Shear Stress)

Below is the link to the video for Demonstration of ANSYS model
https://drive.google.com/file/d/12opyCOPJxGwUfhK2sw_tZopM4QTEOhwz/view

5. References

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