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subject: Exemplar for simulation challenges: Large-deformation micromechanics of Sylgard® 184/glass microballoon syntactic foams

Executive Summary

Sylgard® 184/Glass Microballoon (GMB) potting material is currently used in many NW systems. Analysts need a macroscale constitutive model that can predict material behavior under complex loading and damage evolution. To address this need, ongoing modeling and experimental efforts have focused on study of damage evolution in these materials. Micromechanical finite element simulations that resolve individual GMB and matrix components promote discovery and better understanding of the material behavior. With these simulations, we can study the role of the GMB volume fraction, time-dependent damage, behavior under confined vs. unconfined compression, and the effects of partial damage. These simulations are challenging and push the boundaries of capability even with the high performance computing tools available at Sandia. We summarize the major challenges and the current state of this modeling effort, as an exemplar of micromechanical modeling needs that can motivate advances in future computing efforts.

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1 Key Challenges for Finite Element Micromechanics Simulations

Micromechanics models of the Sylgard®/GMB material explicitly resolve the material meso-structure and allow us to study how damage evolution and local GMB interactions contribute to the global material response under large compressive strains. Key challenges are summarized here:

- Automated generation and meshing for complex microstructure geometry.
  - Sophisticated particle packing algorithms needed to generate microstructures with GMB volume fractions $> 30\%$.
  - GMBs must use quadrilateral shell elements. Prohibitively large numbers of solid elements are needed to resolve the GMB wall thickness ($\sim 1\mu$m) with adequate physics.
  - Meshes must be of sufficient quality for analysis—GMBs cannot touch or overlap, requires a minimum spacing for meshable matrix ligaments.
- Nonlinear material behavior: Sylgard® matrix is viscoelastic/rubbery at room temperature, GMBs need a failure model.
- Inclusion of relevant physics needed to capture GMB failure produces numerical challenges—pushing the limit for current FEA capabilities.
  - Pervasive contact
  - Very large deformations (regime of interest up to 60% macroscale strain)
  - Mesh dependent failure of GMBs
  - Many matrix element inversions occur when GMB failure begins
  - Need to mimic quasi-static behavior using explicit time integration, as implicit solvers cannot converge when GMB failure begins
  - Periodic boundary conditions needed to keep SVE size reasonable and allow GMBs to intersect the SVE boundaries (needed to achieve high GMB volume fractions)

2 Current Approach and Status

The following sections give a brief summary of our current modeling approach and how well it addresses these challenges. The meshing approach and material models have been used successfully to simulate the elastic, small strain behavior of Sylgard®/GMB materials without failure [1]. Simulating large-deformation behavior with multiple GMB failures remains a significant challenge.

2.1 Microstructure and Mesh Generation

Unique microstructure geometries with randomized GMB locations within a cube-shaped stochastic volume element (SVE) are created for many different material configurations. A custom-built Python wrapper code is used in conjunction with existing Sandia tools. The LAMMPS software is used to generate the size distribution and locations for a user-specified GMB volume fraction

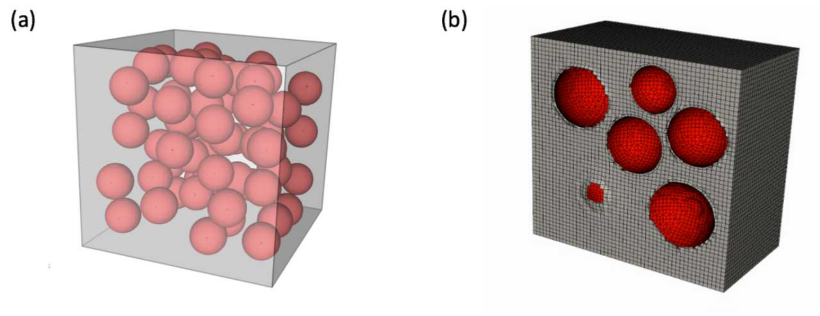

Figure 1. (a) Microstructure model, (b) Cross section of an all-hex mesh generated with Sculpt.

and number of particles. The GMBs are kept from touching each other by enforcing a minimum spacing distance of 3-4 μm. The Sculpt meshing feature [2, 3] in CUBIT is then used to generate an all-hex mesh of the irregular microstructure without requiring any geometry decomposition. The result is the porous matrix structure meshed with solid hex elements, a layer of shell elements representing each hollow GMB, and a void region with no elements inside each GMB structure (Figure 1). Several approaches can be used at the interface between the GMB shell elements and the matrix elements, but the most robust is to require shared nodes.

2.2 Material Models Used for Sylgard® 184 and Borosilicate Glass

A linear viscoelastic representation for Sylgard® 184 adopted from reference [4] is used with the Sierra/SM Universal Polymer Model. Details on this material model are available in [5].

The GMBs are modeled using the Sierra/SM Multilinear Elastic-Plastic Hardening Model with Failure, which is modified to approximate a brittle failure mechanism. Isotropic elastic constants for borosilicate glass are taken from [6][7]. We do not have a clear picture of how borosilicate glass fails at the length scale of the GMB wall thickness ($\sim 1\mu$m), because the fracture behavior of brittle materials is determined by the distribution of inherent flaws. We expect inherent flaws in the GMB walls to be small and the effective fracture strength of the material to be large. Thus, we estimated the yield stress to be 1220 MPa, which is 2% of the Young's modulus for borosilicate glass and use this as a metric to qualitatively observe failure of the GMBs in this microstructure. GMB breakage is accomplished through element death when all the shell integration points fail. The failure is spread out over a 2% equivalent plastic strain to reduce the sensitivity of the microstructure to sudden changes in element behavior. This critical crack opening strain is used purely for model purposes and should not be interpreted as physical.

2.3 Finite Element Simulations–Large Deformation

Large deformation simulations incur the many numerical challenges associated with pervasive GMB failure discussed in Section 1. A short summary of details and assumptions are given here:

- We simulate uniaixial compression using 1/8 symmetry boundary conditions and an applied displacement. We have not yet been successful using periodic boundary conditions with explicit time integration.

- The Explicit Quasistatic Mode capability in Sierra/Solid Mechanics [8] is used to provide a robust computational platform that can model complex mechanisms with which implicit solvers often have difficulty, including large localized deformations and pervasive contact.
- Our failure criterion for GMBs is estimated, and failure is achieved by element death.
- Any matrix elements that invert during the simulation are killed using element death. This was necessary to accommodate failure of multiple GMBs in a single simulation. The matrix elements neighboring failed GMBs commonly invert, and this is an ongoing issue.
- Self-contact was specified for the Sylgard ® matrix to prevent artificial overlap of the matrix ligaments as the GMBs fail. We do not include contact between the GMB shell elements, with the assumption that artificial overlap of the GMBs is negligible compared to matrix deformation. Frictionless contact was used since a reasonable estimate of friction coefficient between matrix ligaments is currently unknown.
- The nominal stress-strain curves become very noisy when GMBs start to fail. We believe this is an artifact of the explicit quasi-static mode numerical methods used and as of yet have not determined its exact cause.
- Without periodic boundary conditions, allowing GMBs to intersect the SVE faces introduces partial GMB structures on the edges. We are unsure how much this affects the global material response, but we anticipate it will be softer than a periodically constrained surface since the partial GMBs on the boundary act like pre-damaged structures.

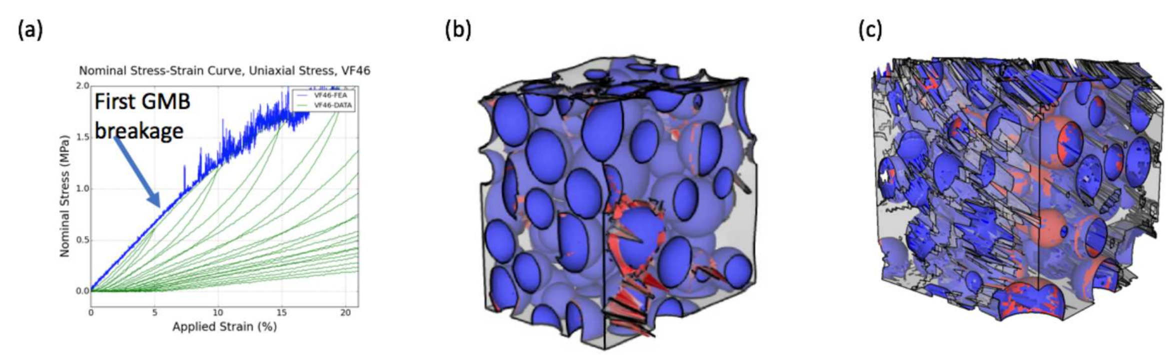

Figure 2. (a) Predicted stress-strain curve compared with macroscale experiment, (b) Deformed state while simulation remains stable (dead shell elements shown in red), (c) Deformed state at last output before simulation failure showing extensive matrix element death.

2.4 Results & Summary

Figure 2 shows the best result we have achieved with this approach. The fundamental shape of the predicted stress-strain curves reflects experimentally measured behavior of Sylgard®/GMB materials, which is promising. However, we can only get up to about 15 - 20% strain before the simulation fails due to pervasive element inversion in the matrix. Future computing efforts that address these challenges would advance our ability to study this and many other materials that have similar mesoscale features.

References

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