Micromechanics-based Determination of Effective Elastic Properties of Polymer Bonded Explosives

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Polymer Bonded Explosives

Polymer bonded explosives are particulate composites. The two primary components of these composites are explosive particles and a rubbery binder. The volume of particles in the composite is typically around 90% of the total volume.

Table 1 Typical polymer bonded explosives.

PBX	Particles Material	Particles Vol. Frac	Binder Material	Binder Vol. Frac
PBX 9010	RDX	0.87	KEL-F-3700	0.13
PBX 9501	HMX	0.92	Estane/BDNPA-F	0.08
PBX 9502	TATB	0.90	KEL-F-800	0.10

PBX 9501 contains 92% by volume of HMX (high melting explosive) particles and 8% by volume of binder. The HMX particles are monoclinic and linear elastic. The binder is a 1:1 mixture of the rubber Estane 5703 and a plasticizer (BDNPA/F). The mechanical behavior of the binder is strain rate and temperature dependent. As a result, the response of PBX 9501 also depends on strain rate and temperature.

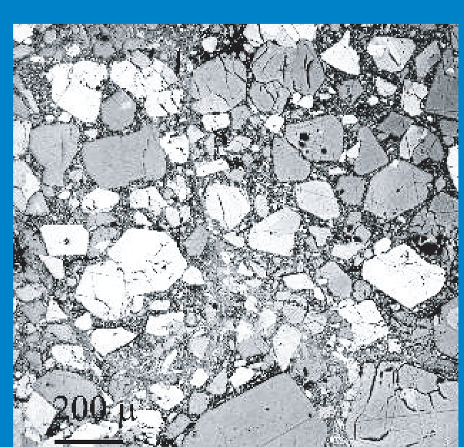

Figure 1 Microstructure of PBX 9501.

Table 2 Elastic properties of HMX.

Young's modulus (GPa) Expt.	Young's modulus (GPa) MD Simulation	Poisson's ratio Expt.	Poisson's ratio MD Simulation
15.3	17.7	0.32	0.21

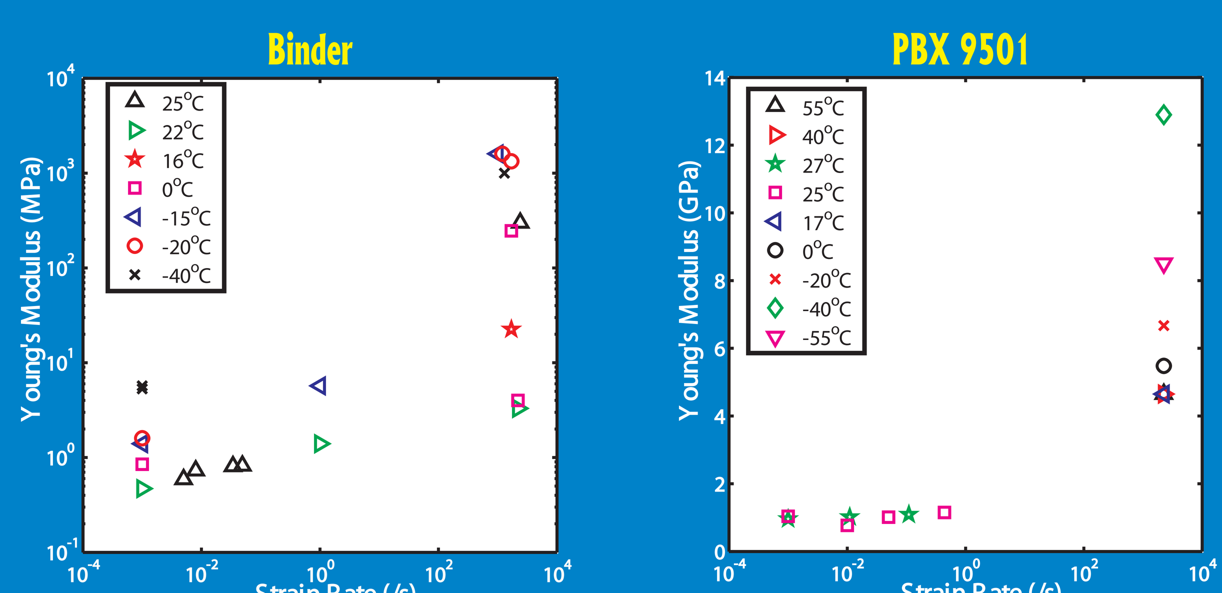

Figure 2 Young's modulus of binder and PBX 9501. Poisson's ratio is 0.49 for the binder and 0.35 for PBX 9501.

Micromechanics

- Exact Relations
- Third-Order Bounds
- Differential Effective Medium (DEM)
- Finite Element (FEM) Approximations
- Generalized Method of Cells (GMC)
- Recursive Cell Method (RCM)

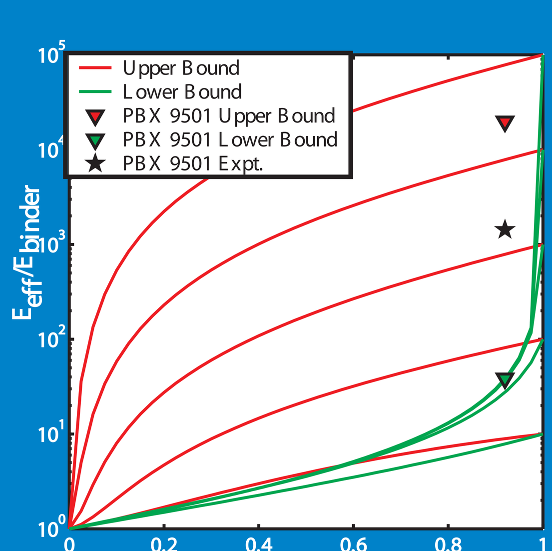

Figure 3 Third-order bounds and PBX 9501.

Exact relations and DEM are used to assess the accuracy of FEM and RCM. Bounds can be observed to be widely separated. Direct GMC does not model stress bridging accurately.

In the recursive cell method (RCM) the representative volume element (RVE) is divided into a regular grid of subcells. Instead of the whole RVE, small square blocks of subcells are homogenized at a time. The procedure is repeated recursively until a single homogeneous material remains. This material is the effective material.

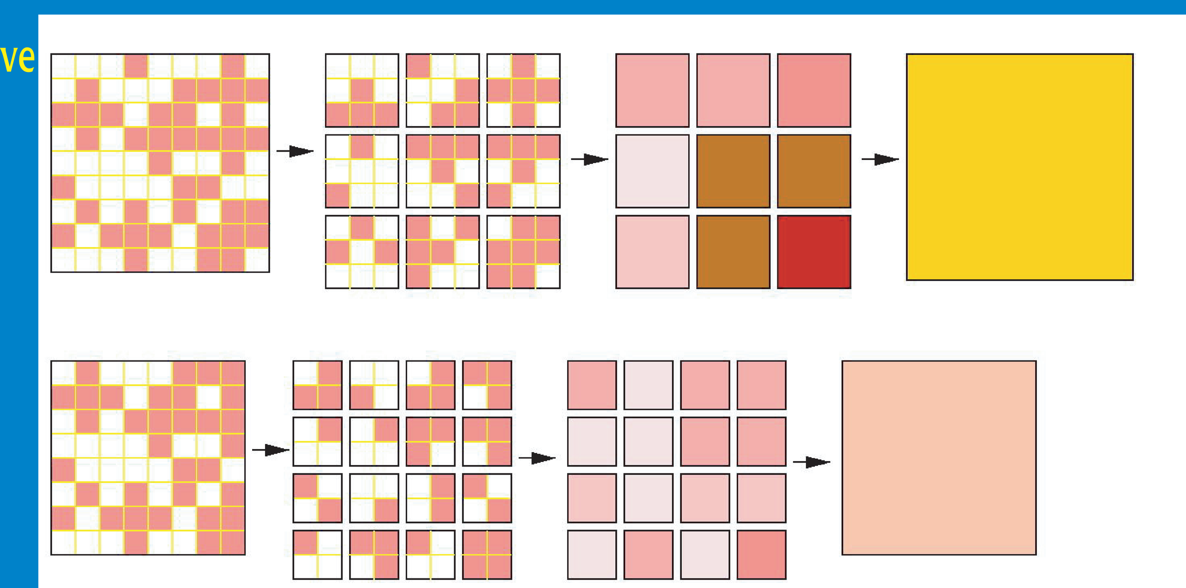

Figure 4 Schematic of recursive cell method (RCM).

Modeling Particulate Composites

Figure 5 Model particulate composite microstructures.

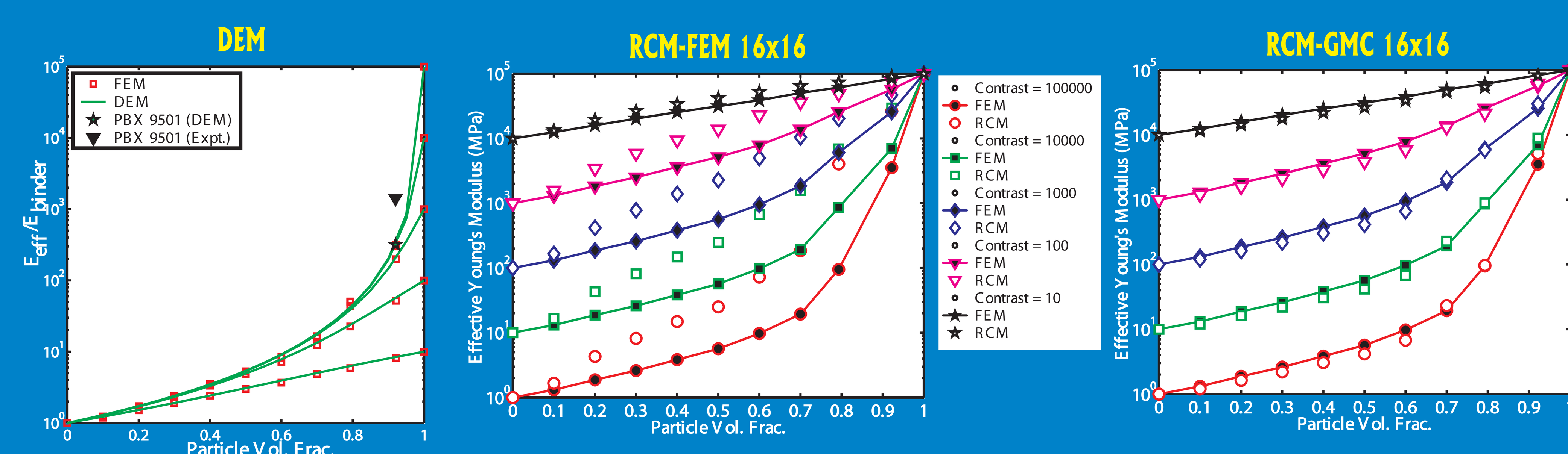

Figure 6 Differential effective medium (DEM), Recursive Cell Method with FEM homogenizer (RCM-FEM), and Recursive Cell Method with GMC homogenizer (RCM-GMC) vs. finite element estimates.

Three-D. vs. Two-D:

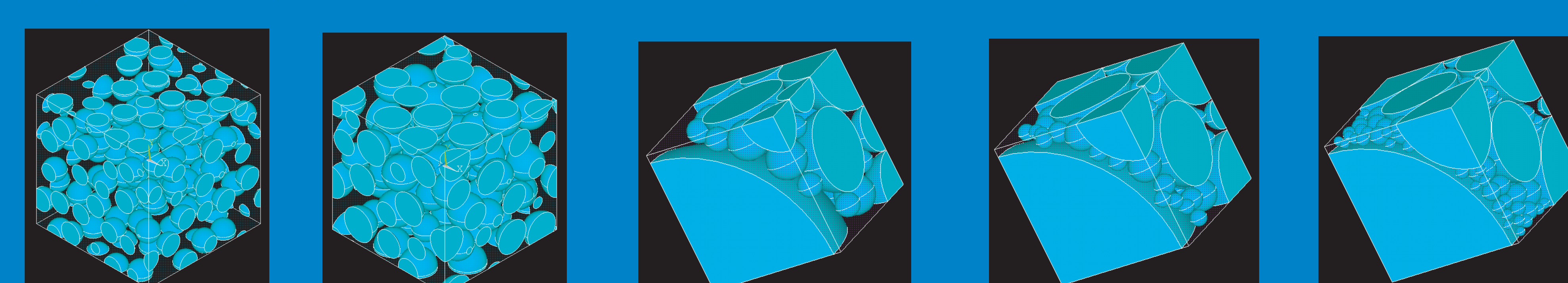

Figure 7 Three-dimensional models of particulate composites.

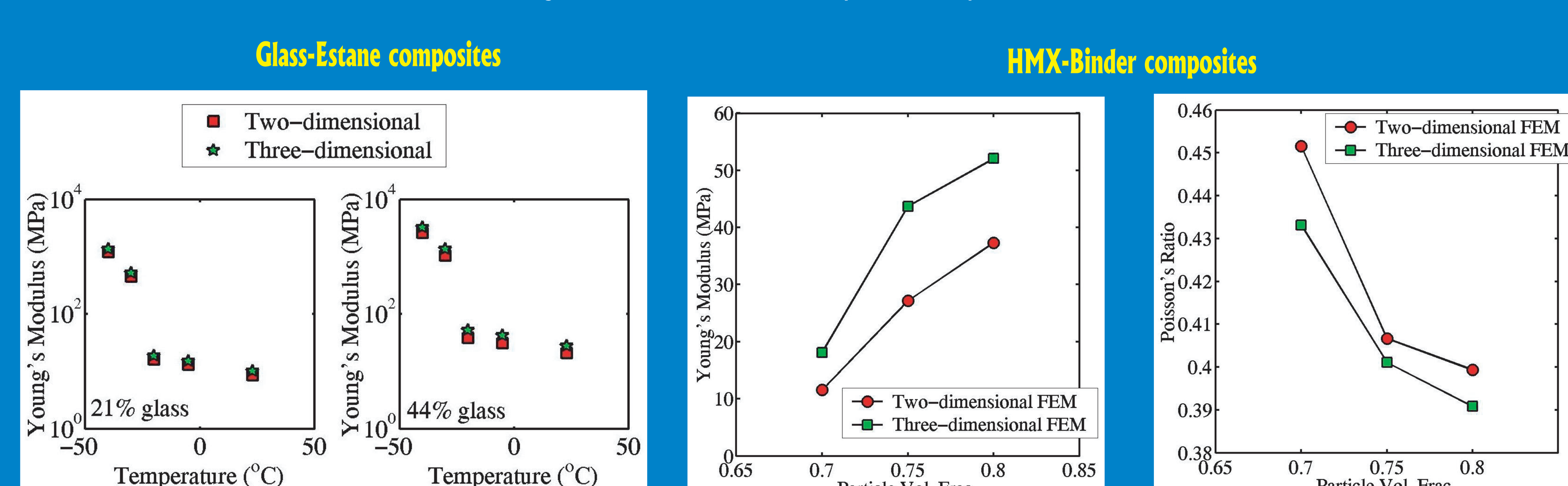

Figure 8 Three-dimensional vs. two-dimensional finite element estimates.

-- Two-dimensional finite element estimates are close to differential effective medium predictions.
-- RCM-GMC estimates closer to finite element estimates than RCM-FEM predictions.
-- Difference between two- and three-dimensional finite element estimates is small.

Modeling PBX 9501

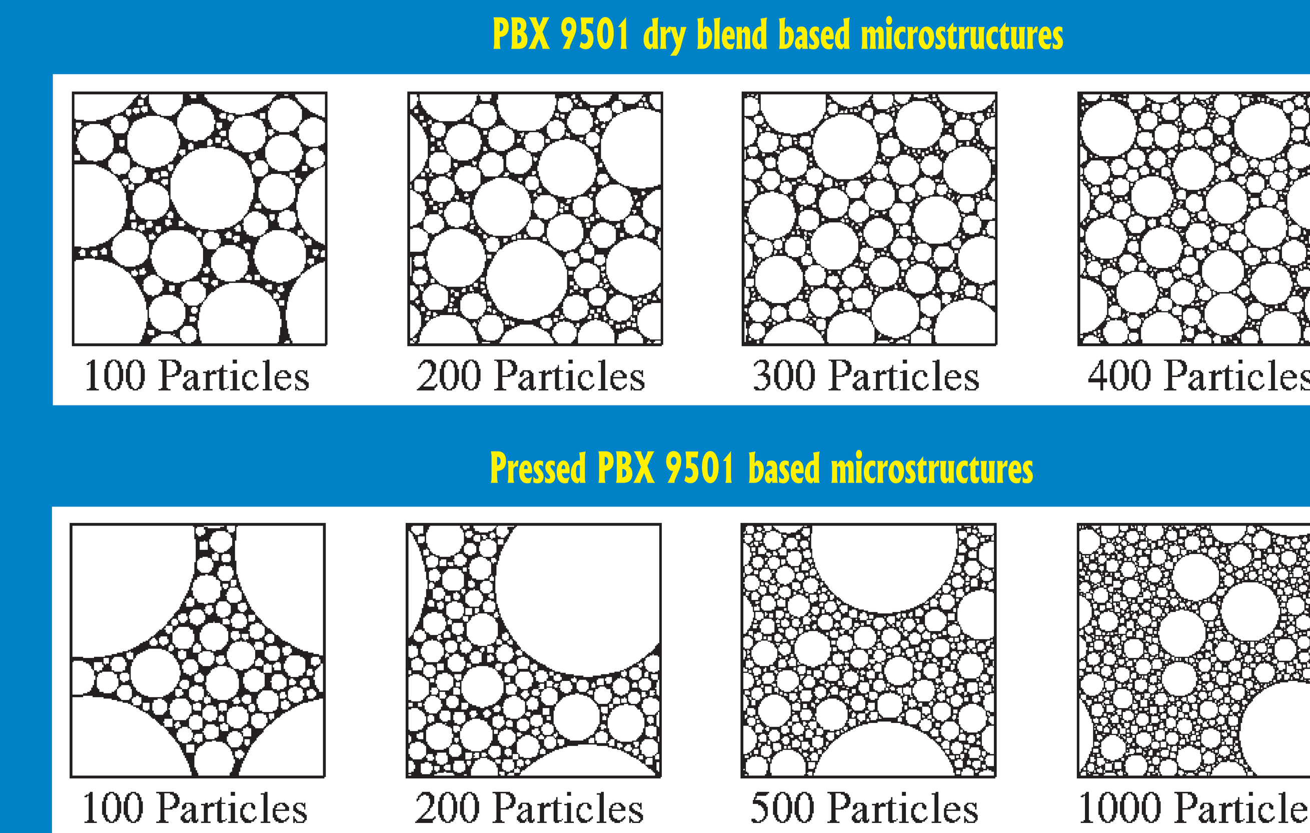

Figure 9 Models microstructures representing PBX 9501.

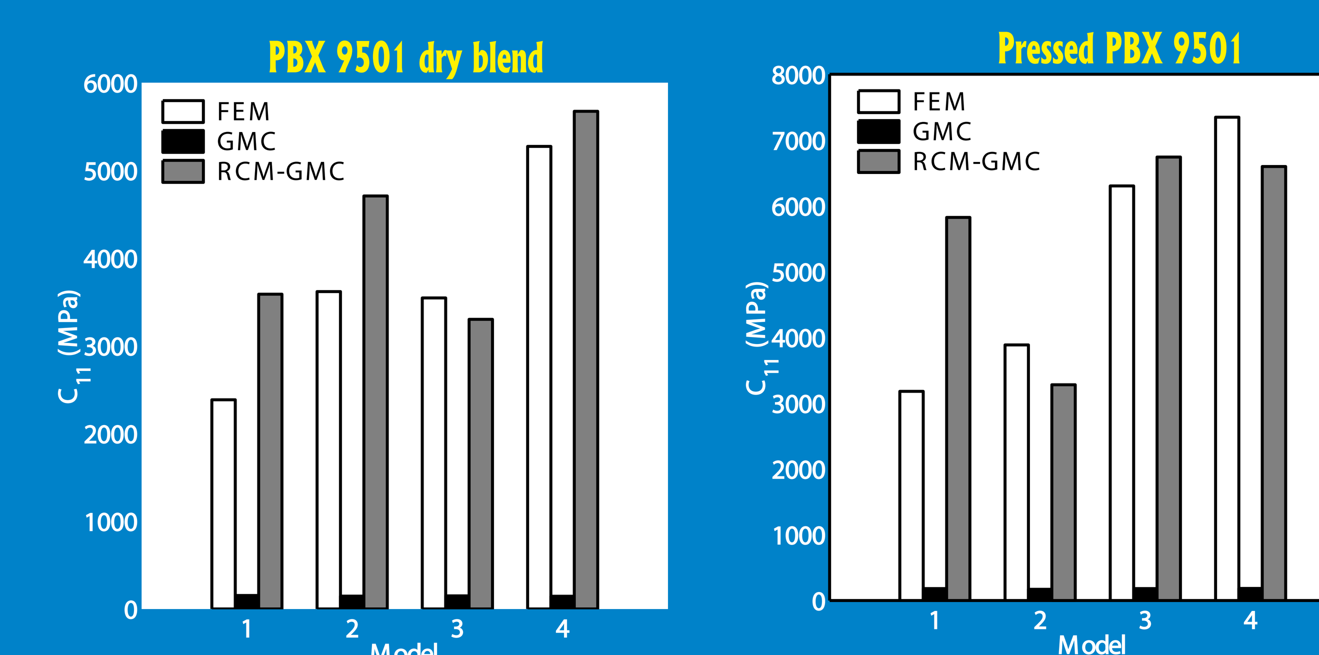

Figure 10 Effective properties of model RVEs from FEM, GMC, RCM-GMC.

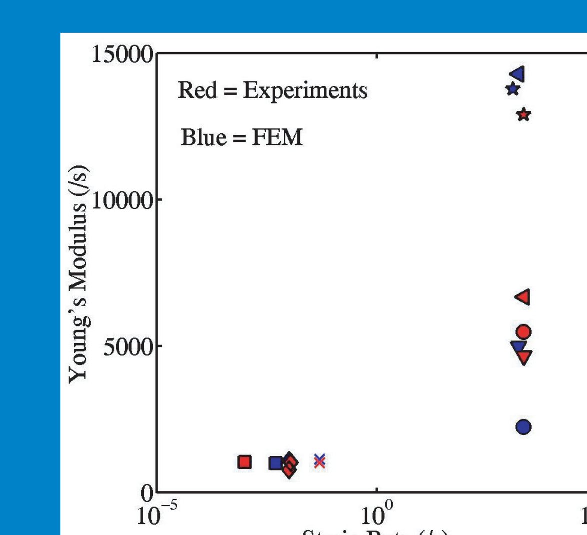

Figure 11 Finite element prediction vs. experimental data on the Young's modulus of PBX 9501.

Conclusions

- Predicted effective properties are strongly microstructure dependent.
- Detailed numerical simulations are required for accurate estimates.
- Recursive cell method with the generalized method of cells homogenizer can predict effective moduli that are close to finite element estimates with considerably greater computational efficiency.

Acknowledgements
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