Micromechanics of thermoplastic elastomers with random microstructures[1]

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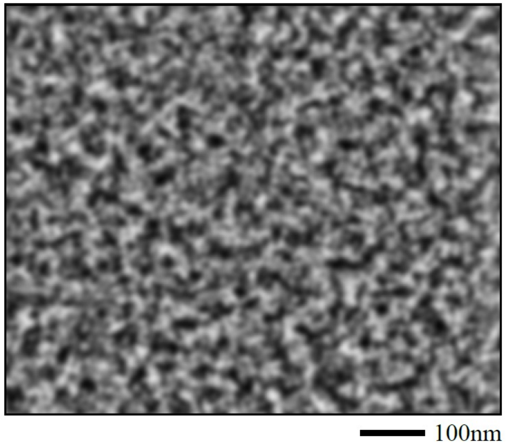
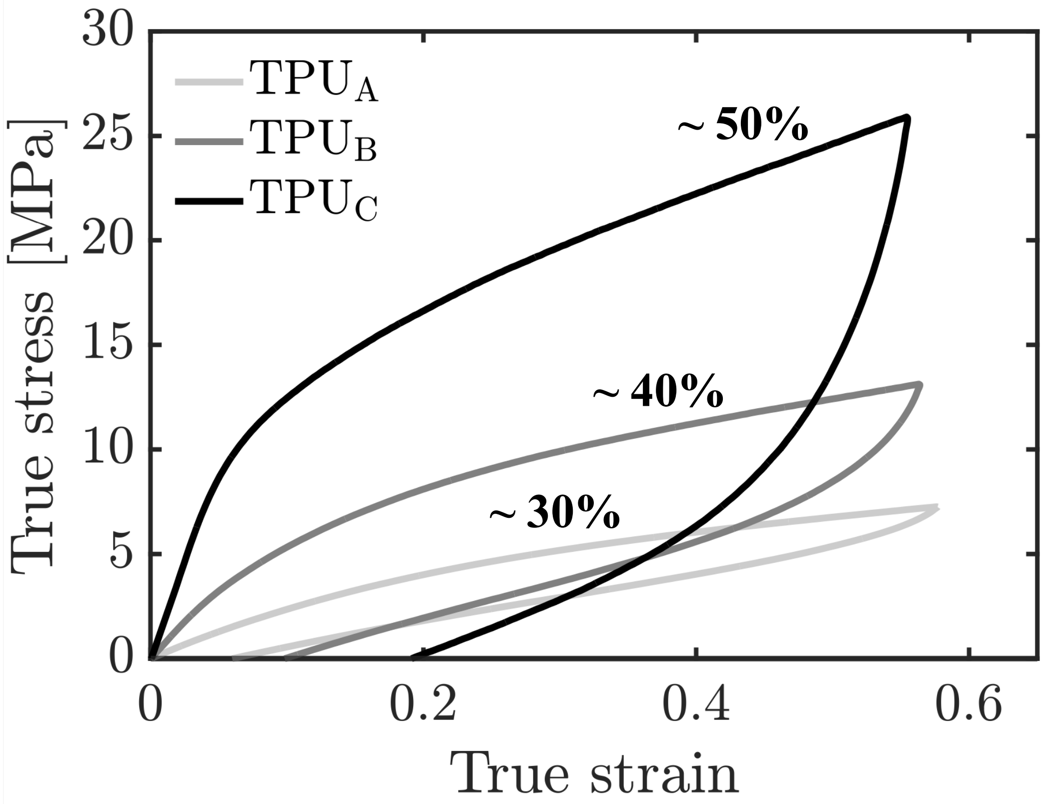
Thermoplastic polyurethanes (TPU)



TEM image[2]



- Block copolymeric materials composed of hard and soft domains[3-5]
- Macro- and micromechanics of "large strain" behavior of thermoplastic polyurethanes (TPU)[1,2]

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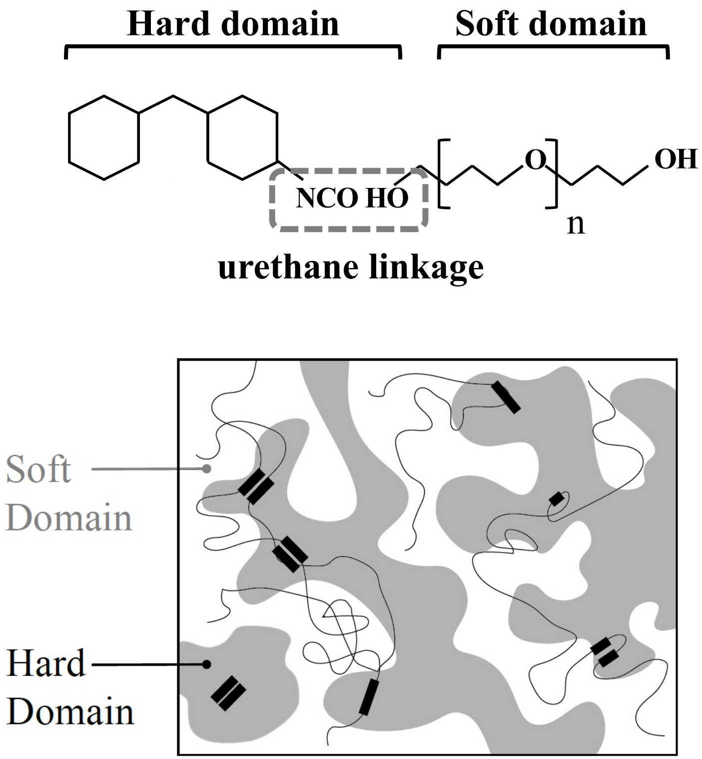

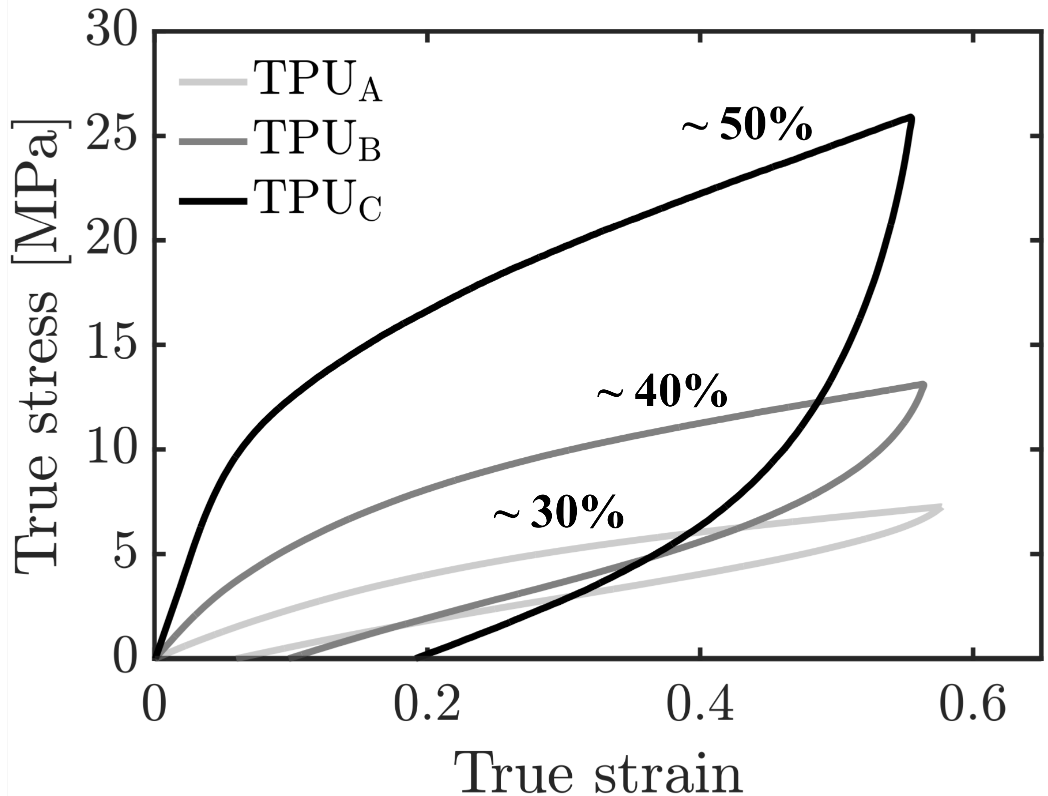

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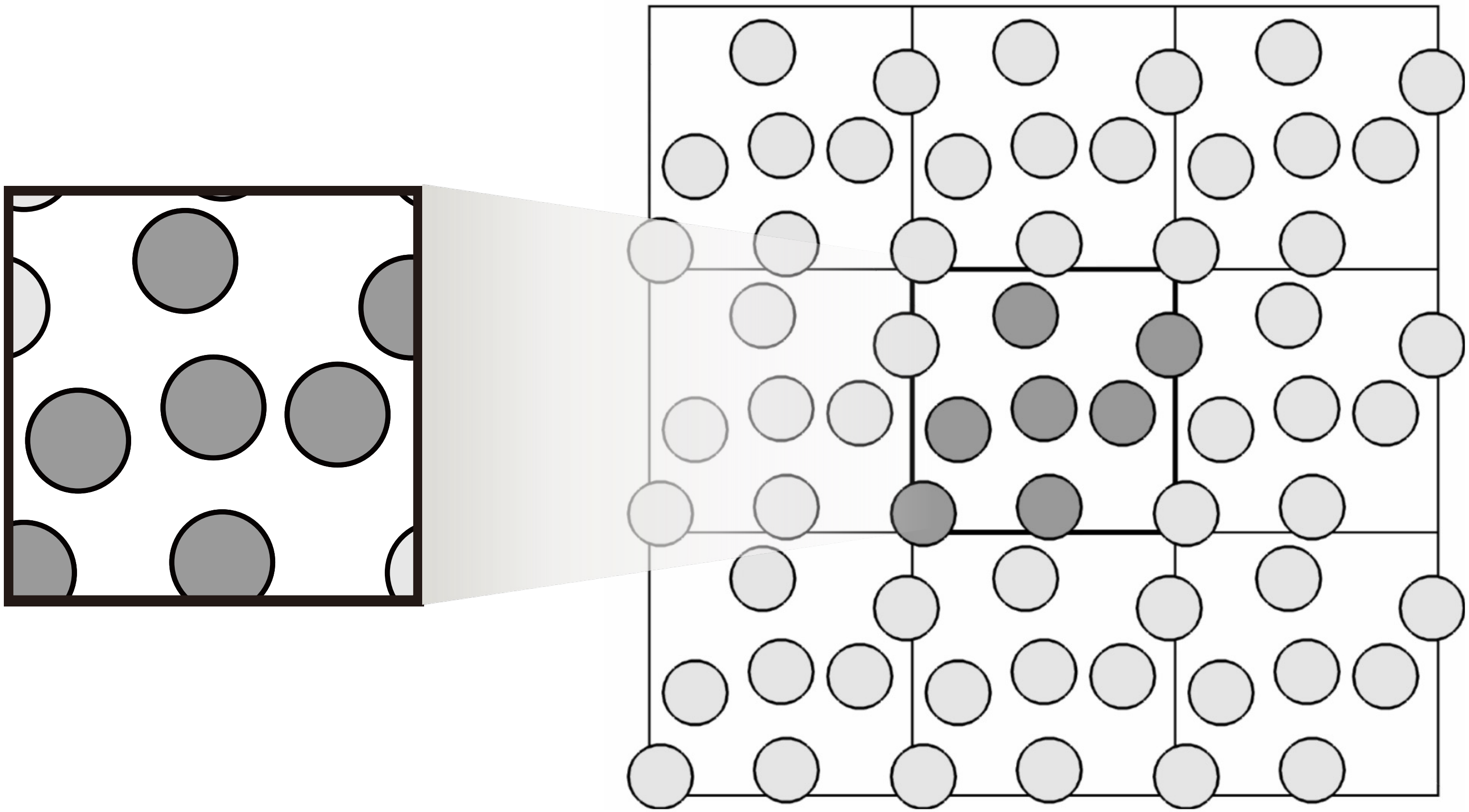
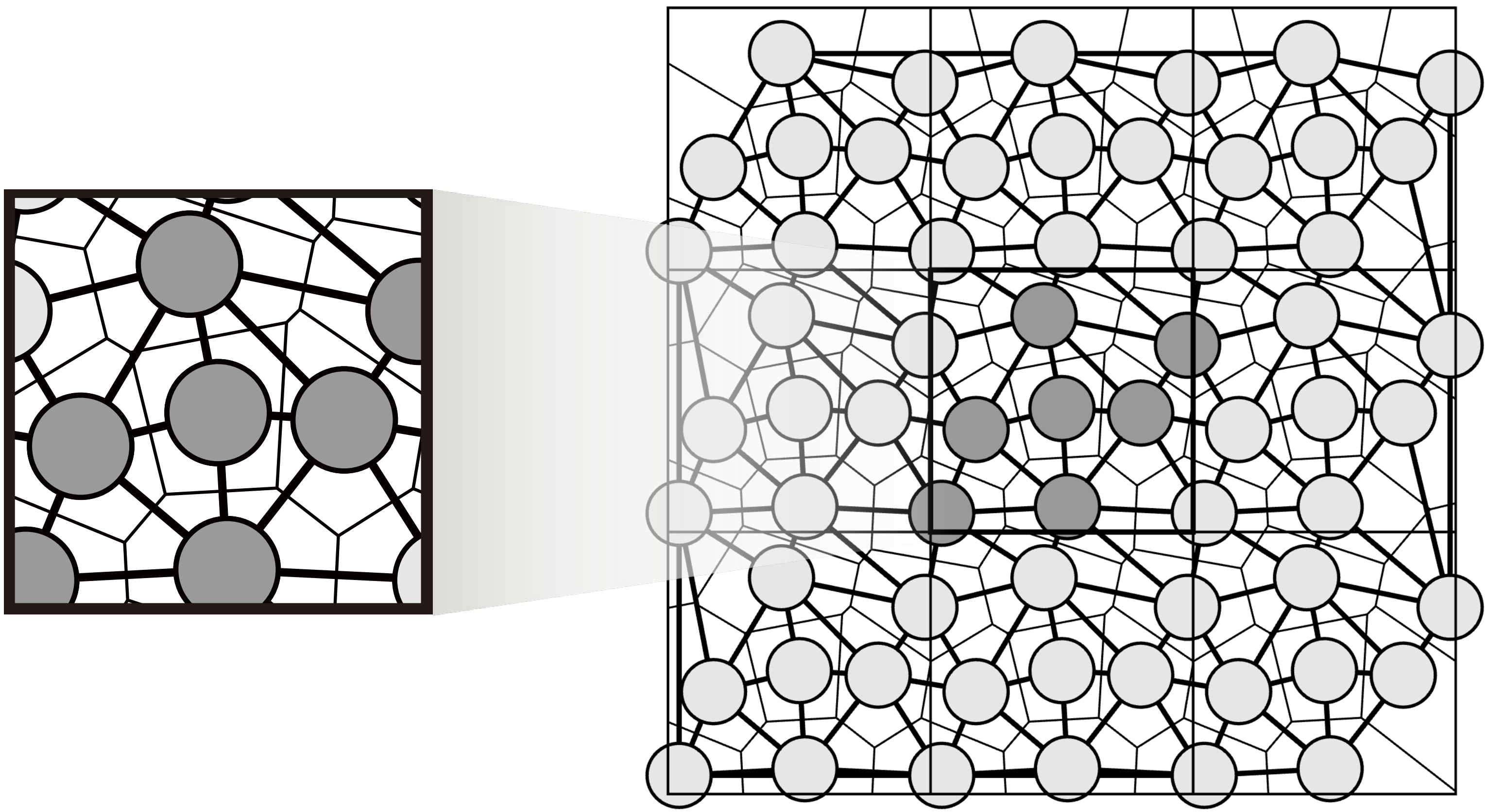
- Macro- and micromechanics of "large strain" behavior of thermoplastic polyurethanes (TPU)[1,2]

Construct "Random" microstructures



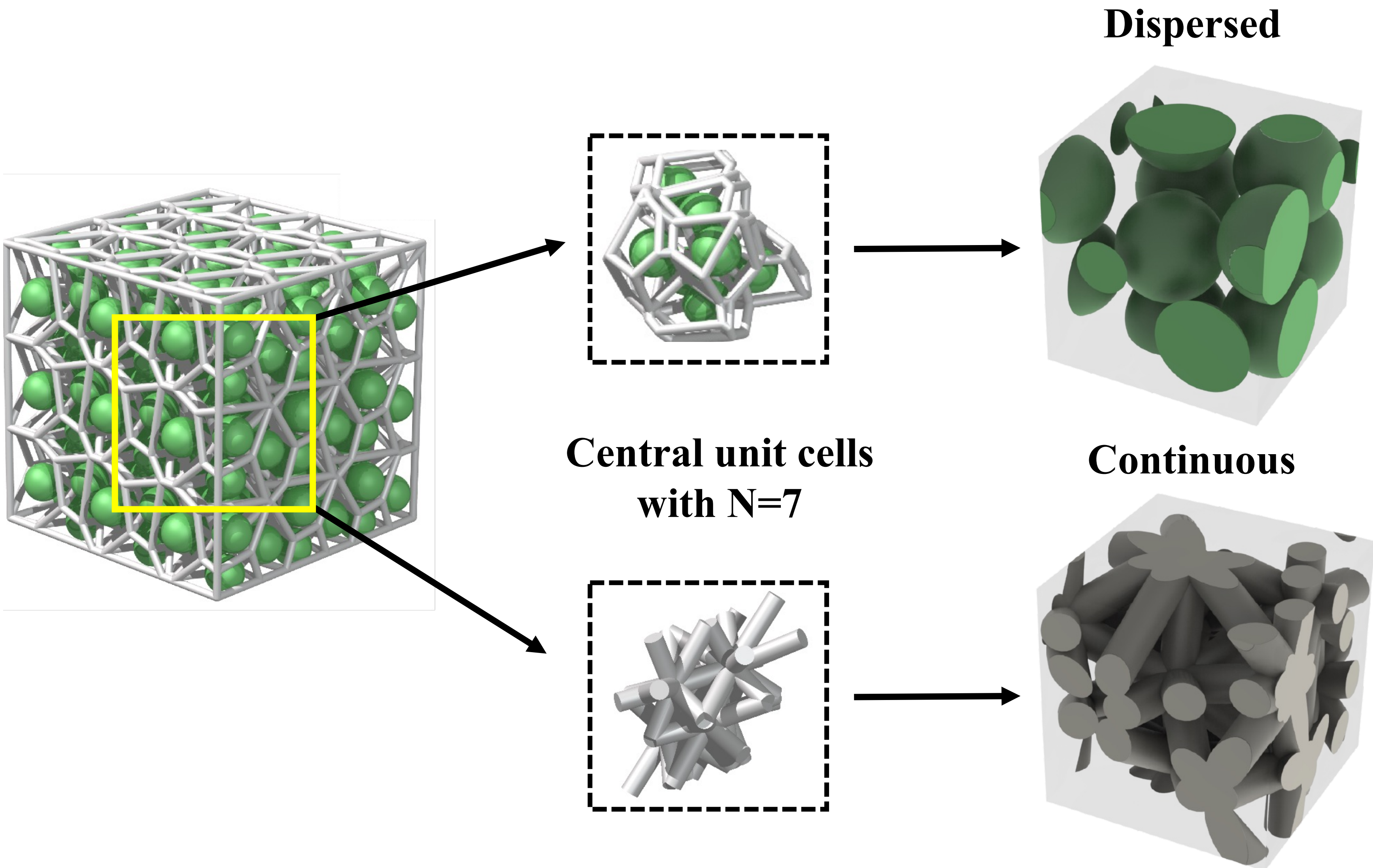
- Random packing of monodispersed spheres in periodic boundary conditions[6,7]

Random spatial points + tessellations



- Identification of the neighbors via Voronoi tessellations[8]
- By connecting with the neighbors → continuous, disordered microstructures available

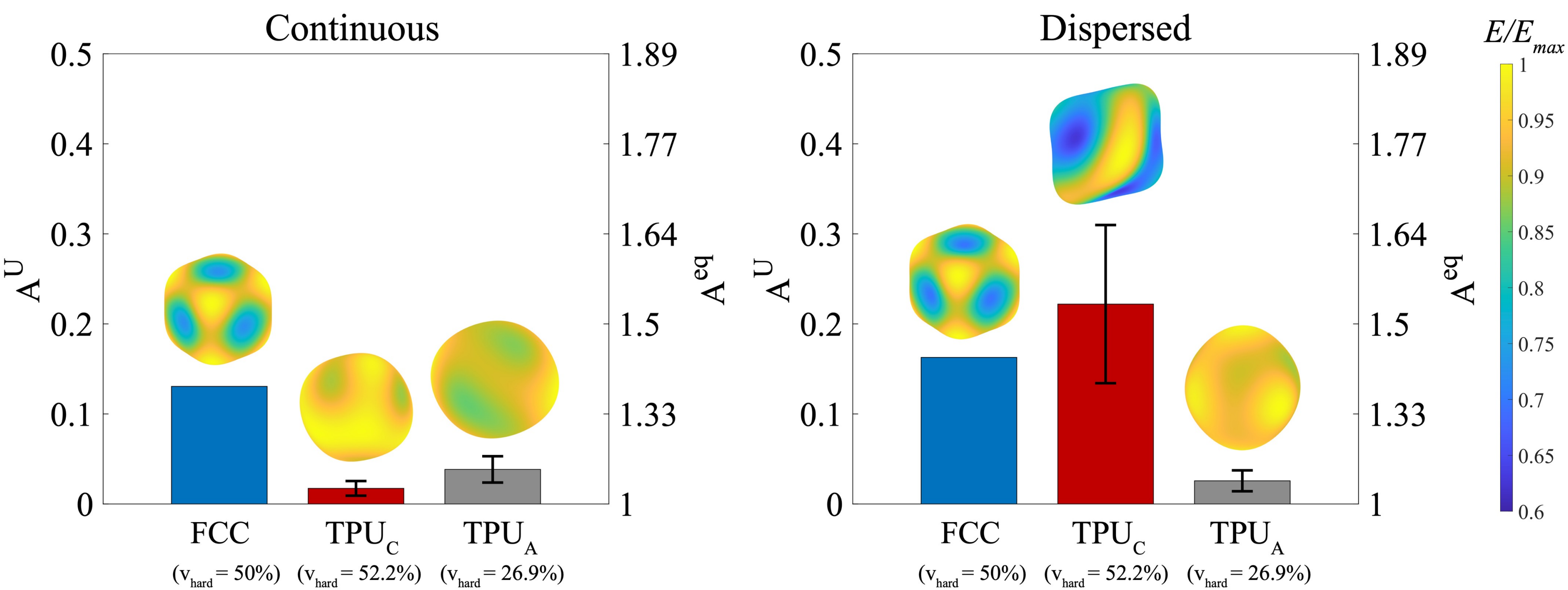
Proposed microstructures: Dispersed vs. continuous



- Only hard domains shown; we constructed two-phase materials

Identification of the N for RVEs

- Elastic anisotropy of both continuous and dispersed morphologies with N=7



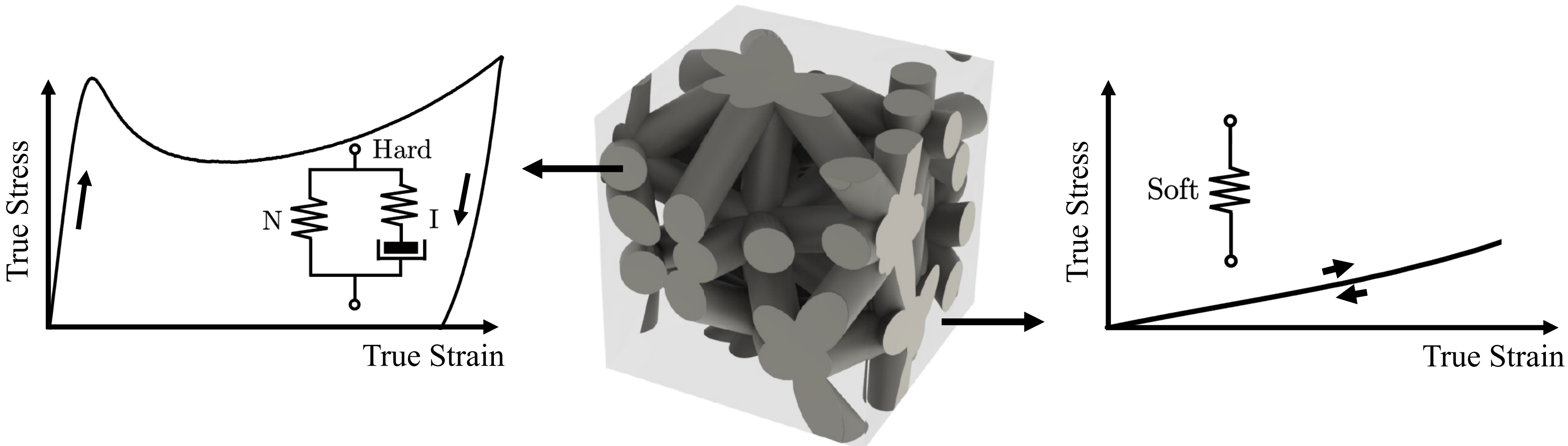
- **Universal anisotropy index**[9,10]

$$A^U = \mathbf{C}^V : \mathbf{S}^R - 6 = 5\frac{G^V}{G^R} + \frac{K^V}{K^R} - 6 \geq 0 \qquad (\text{Isotropic} : A^U = 0)$$

Constitutive behavior of hard and soft domains

Hard: Thermoplastic behavior

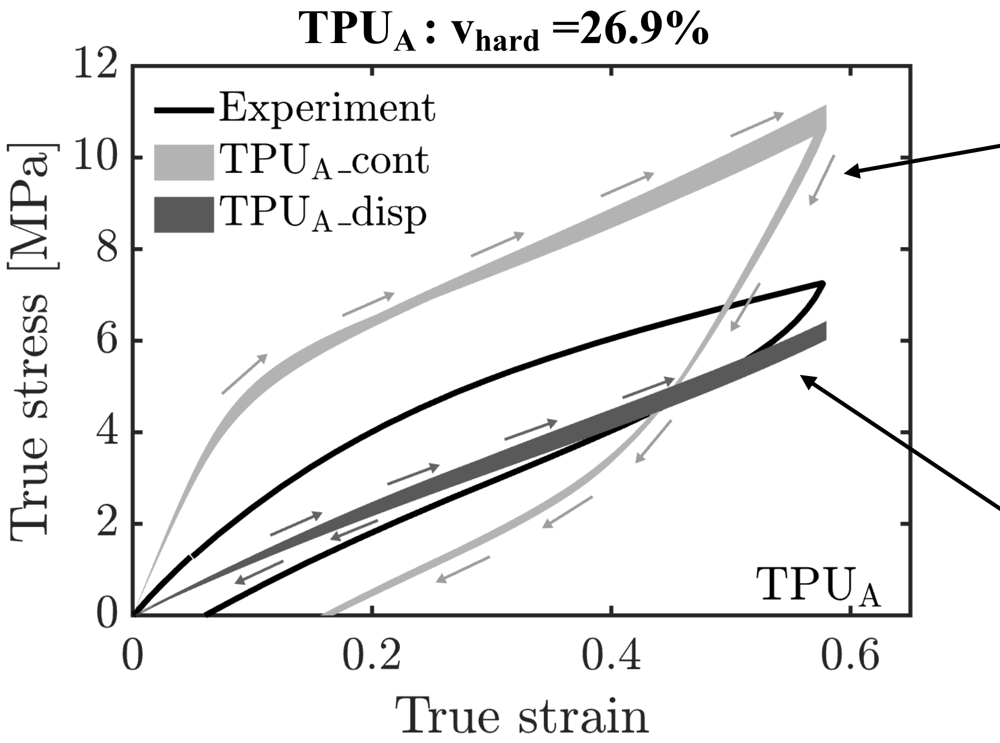
Soft: Elastomeric behavior

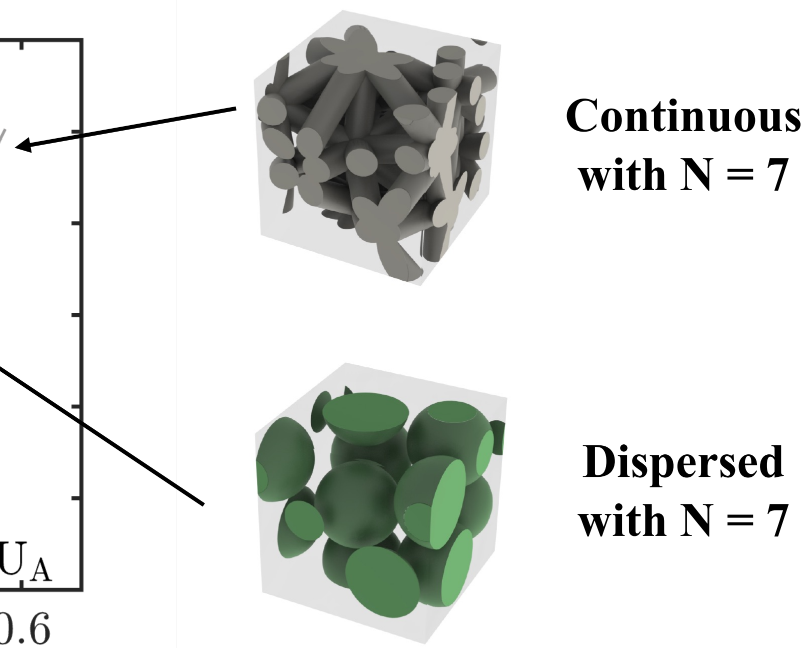


- **High initial stiffness**
- **Energy dissipation**
- **Residual strain**

- **Rubbery-like behavior**
- **Compliance**
- **Resilience**

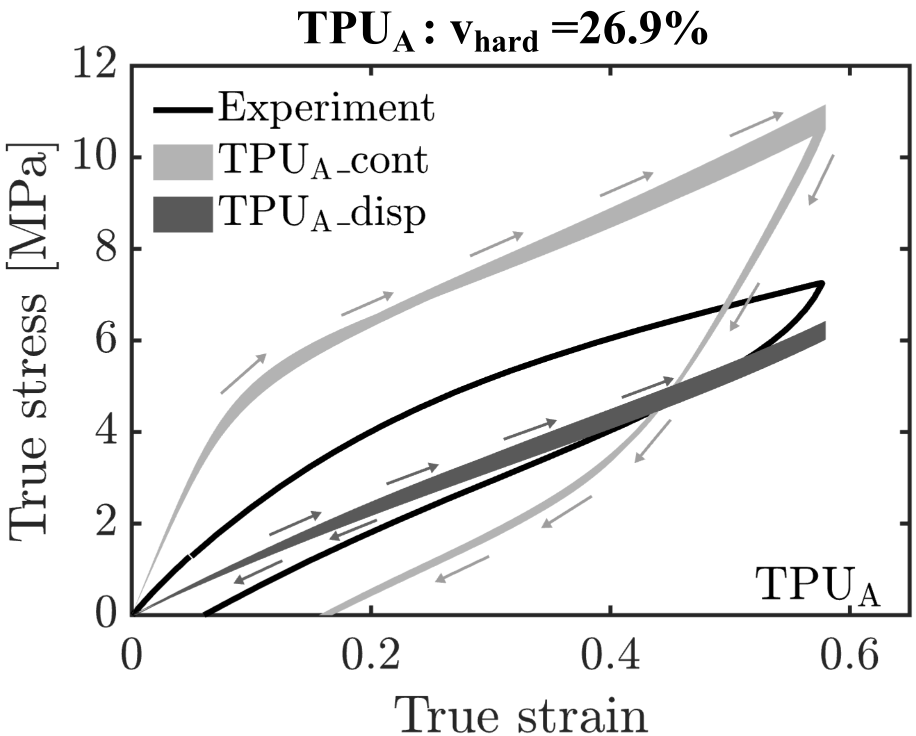
Dispersed vs. continuous: Role of connectivity

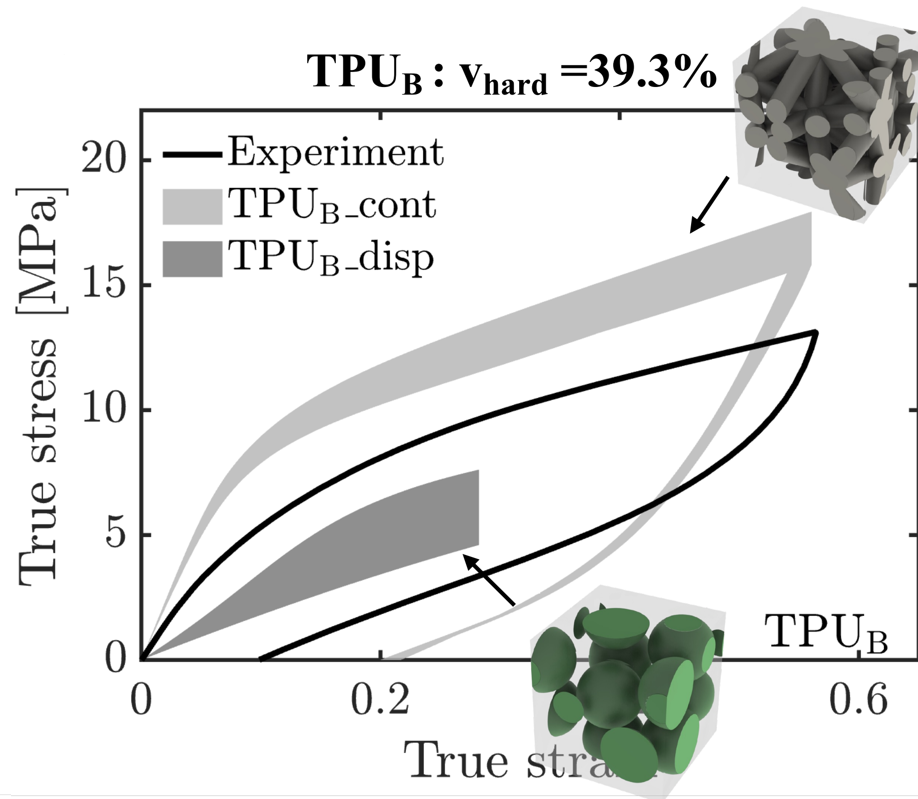




- Greater stress response, stiffer initial modulus, significant energy dissipation in the RVE with continuous hard domain [11,12]
- Numerical simulation results with five statistical realizations

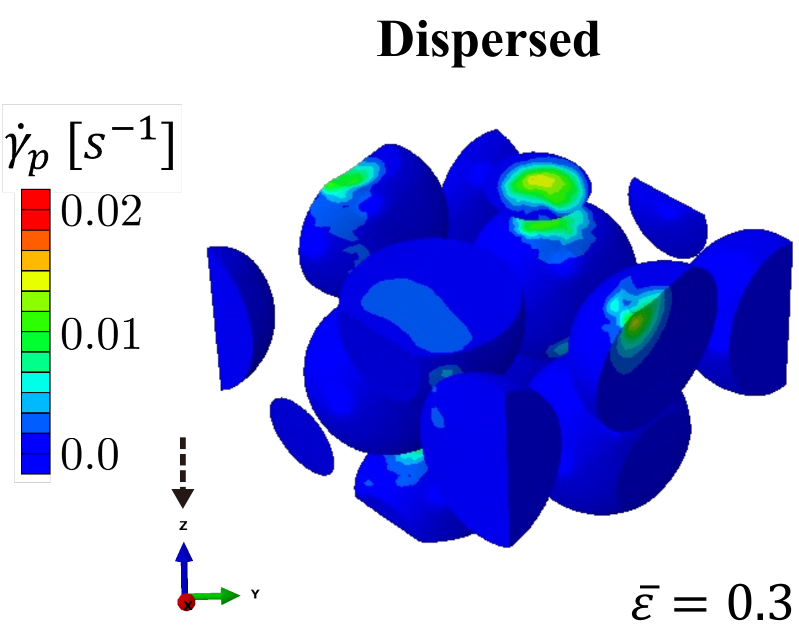
Dispersed vs. continuous: Role of connectivity

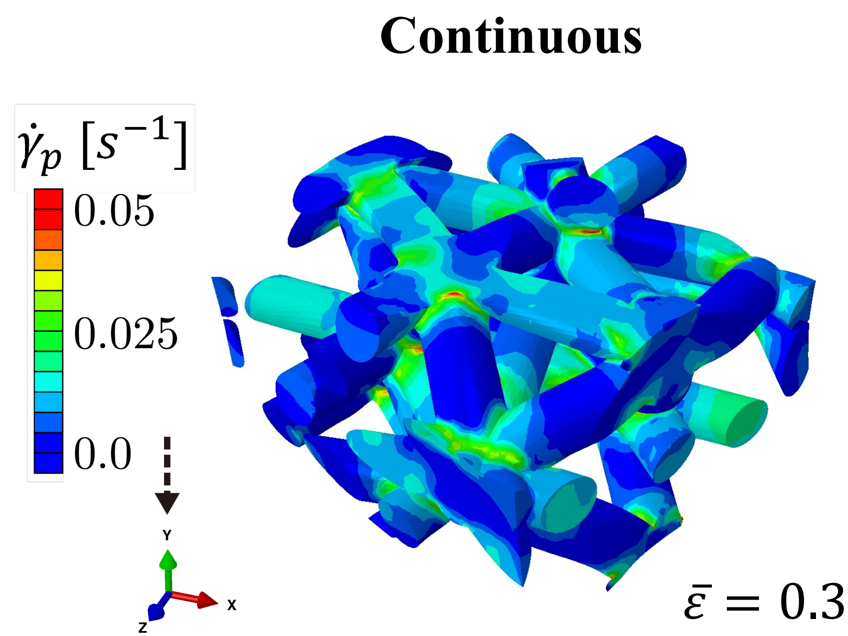




- In case of TPU_B → closer to the stress-strain response with continuous hard domain
- TPU_B (higher volume fraction; **39.3%**) **is likely to possess more "connected" domains**

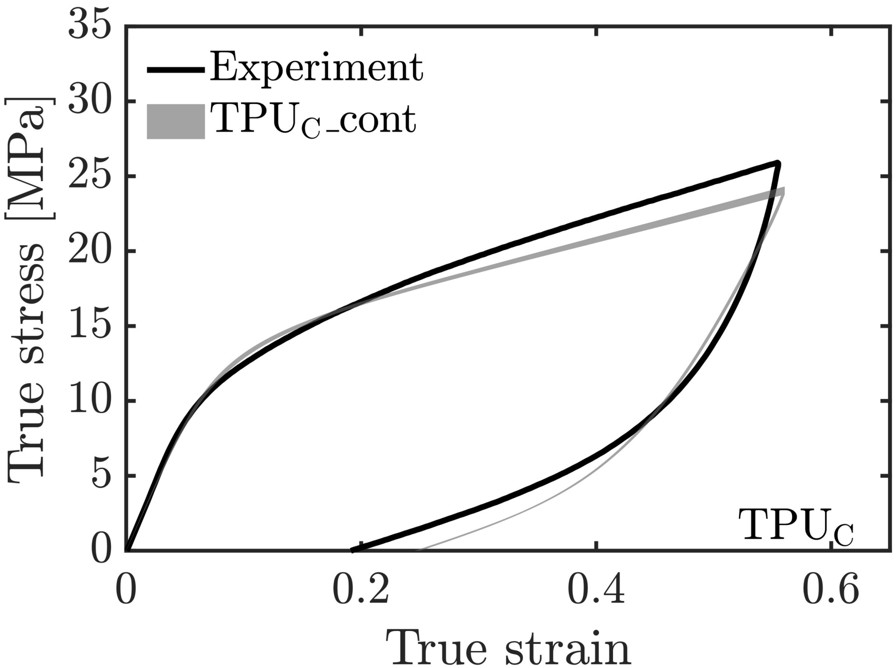
Dispersed vs. continuous: Role of connectivity

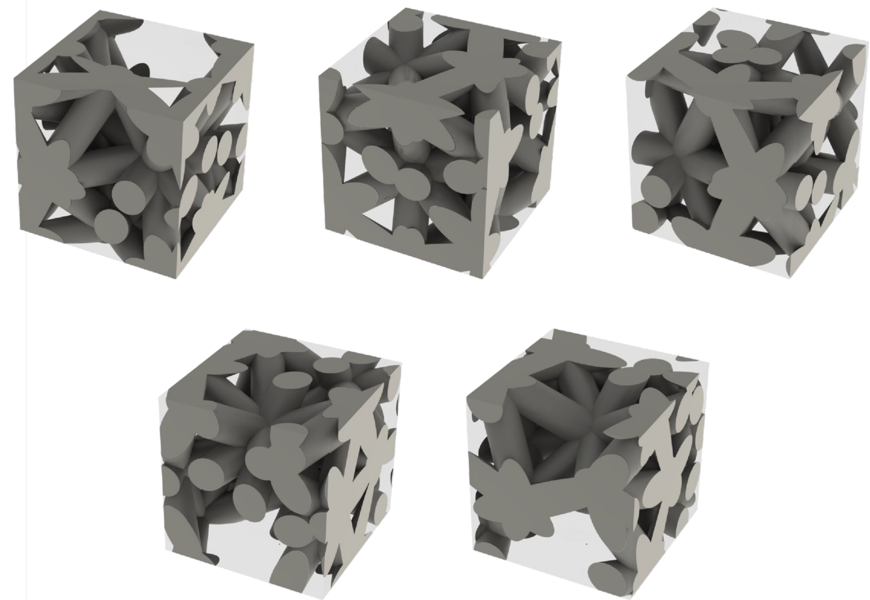




- Contours of plastic flow rates in dispersed and continuous RVEs of **TPU_B (v_{hard} =39.3%)**
- **Plastic flow** developed throughout the hard ligament, which results in the **stress-rollover** in the RVEs **with continuous hard domain**

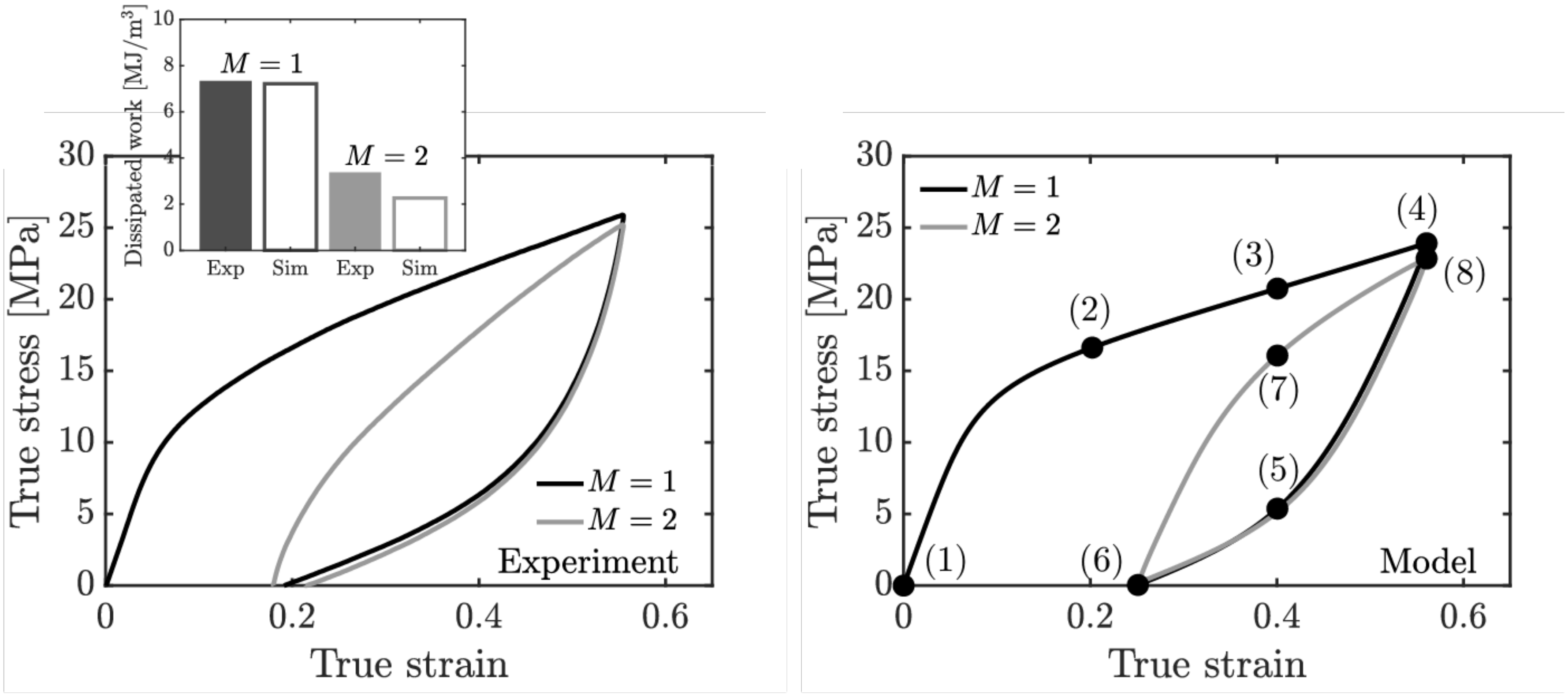
Dispersed vs. continuous: Role of connectivity





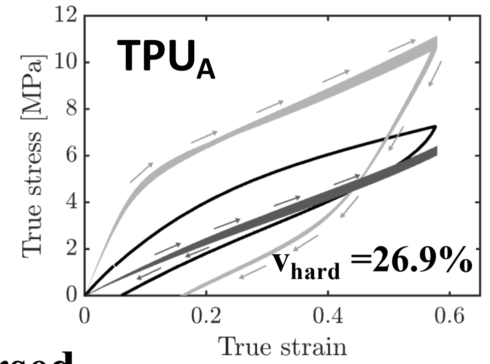
- Micromechanical model with **continuous hard domain** nicely captured the main features of TPU$_C$ with highest volume fraction (**v_{hard} = 52.2%**)

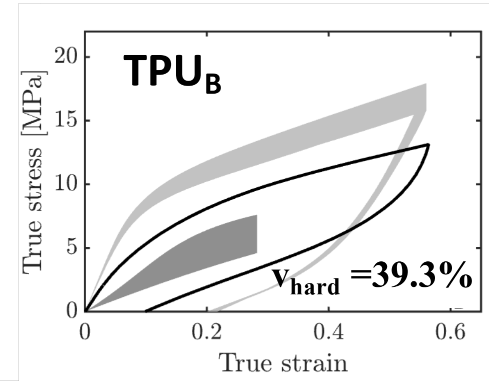
Cyclic loading behavior



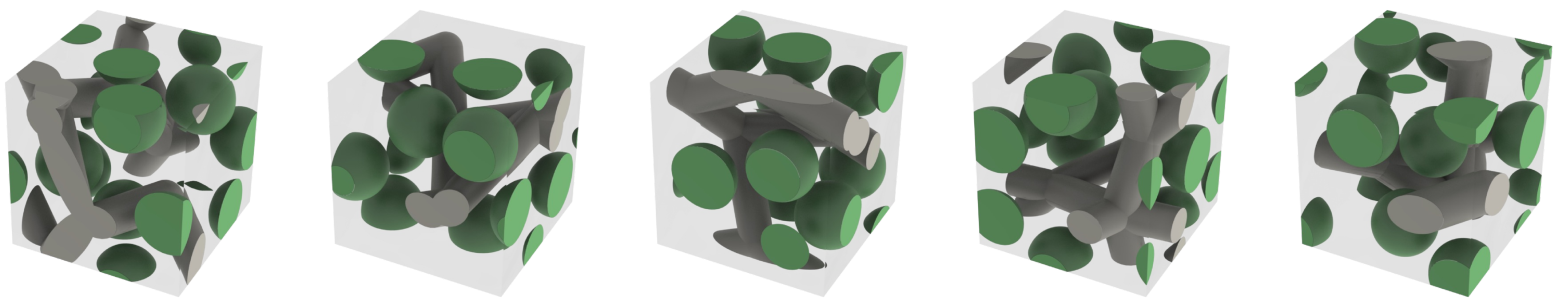
- Stretch-induced softening (Mullins' effect) was clearly manifested in the second cycle and was nicely captured by the micromechanical model[13,14]

"Mixed" RVEs

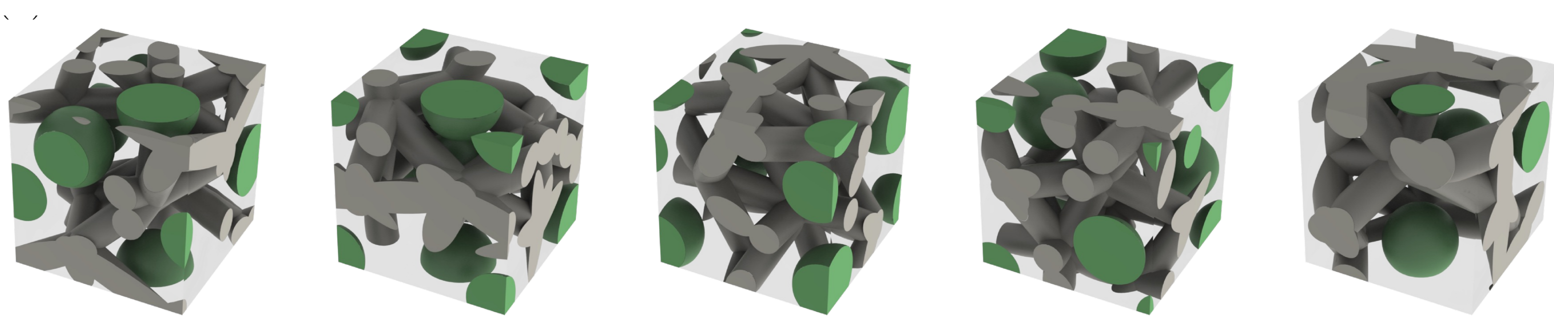




(1) TPU$_A$: 40% continuous / 60% dispersed

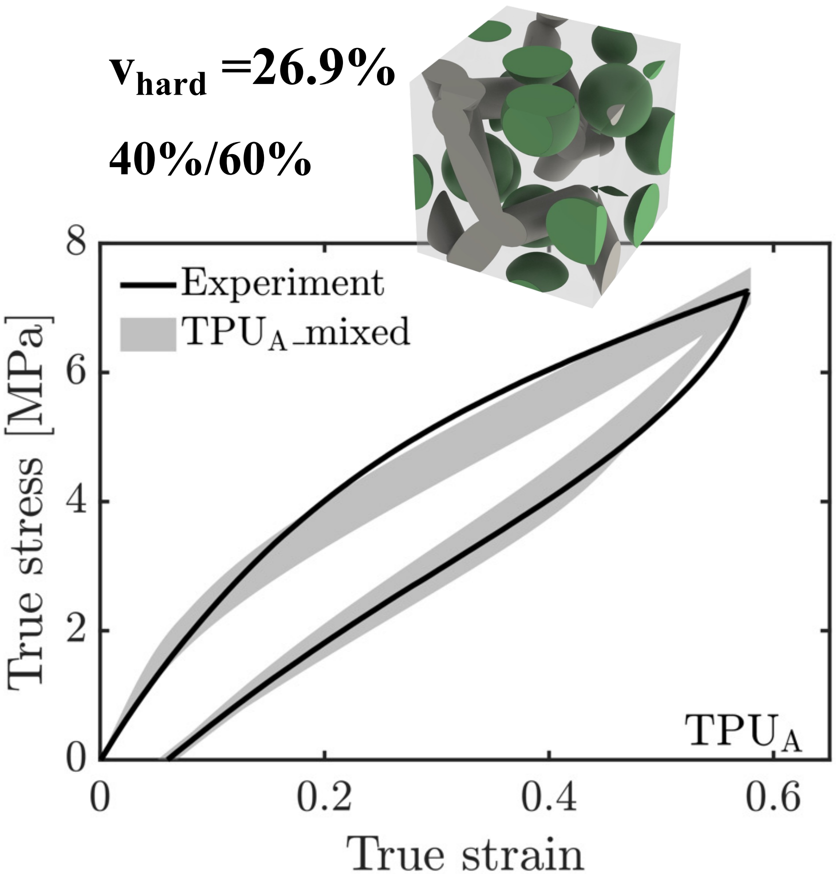


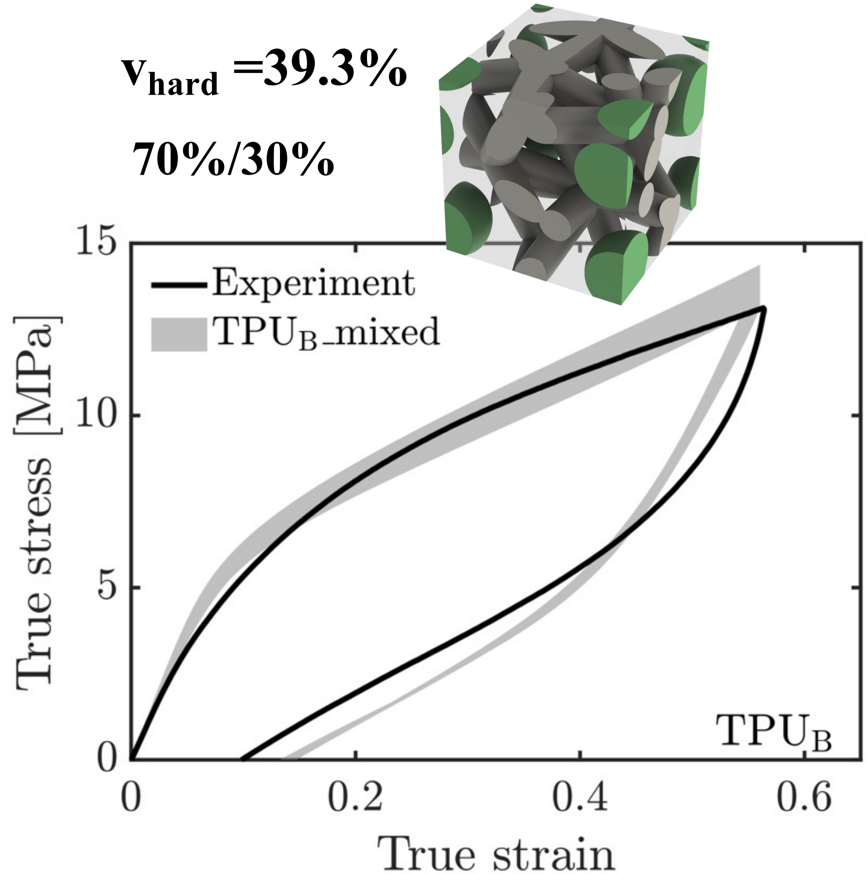
(2) TPU$_B$: 70% continuous / 30% dispersed



- Voronoi points *N*=10

“Mixed” RVEs





- Nicely captured the major features of the experimentally measured stress-strain response

Conclusion and Future works

- Micromechanical modeling of **“two-phase” elastomers** with two different disordered morphologies: **(1) dispersed** and **(2) continuous hard domains**

- **Connectivity** of hard domains impacts key elastic/inelastic features under cyclic loading

- Newly constructed **mixed RVEs →** co-existing dispersed and continuous morphologies

- Useful tool for micromechanical analysis of **“two-phase” materials with random microstructures**

→ Design of topological features for tailoring macroscopic mechanical properties[11,12]

→ Furthermore, explore the fracture behavior in a variety of elastomeric materials[15-18]

Acknowledgement

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