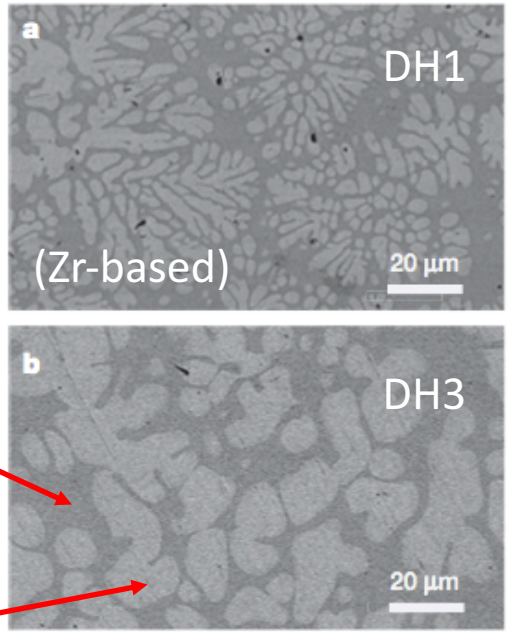
Improving Uniform Plastic Shear Deformation in a Disordered Bidisperse Mixture by Incorporating a Disperse Ordered Phase

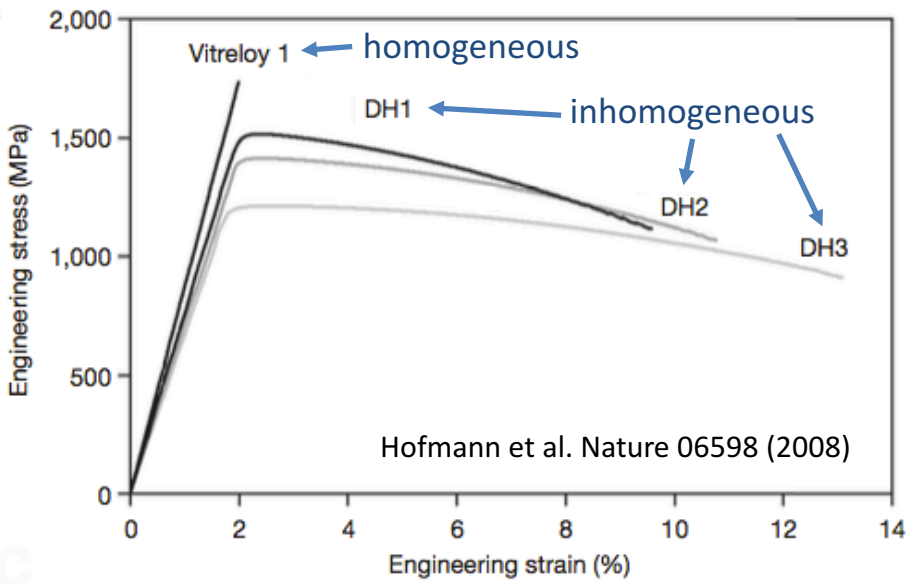
Guo-Jie Jason Gao[1], Yun-Jiang Wang[2,3], Shigenobu Ogata[4,5]

1. Dept. of Mathematical and Systems Engineering, Shizuoka University,
2. State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences,
3. School of Engineering Science, University of Chinese Academy of Sciences,
4. Department of Mechanical Science and Bioengineering, Osaka University,
5. Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University.

metallic glass (disordered)

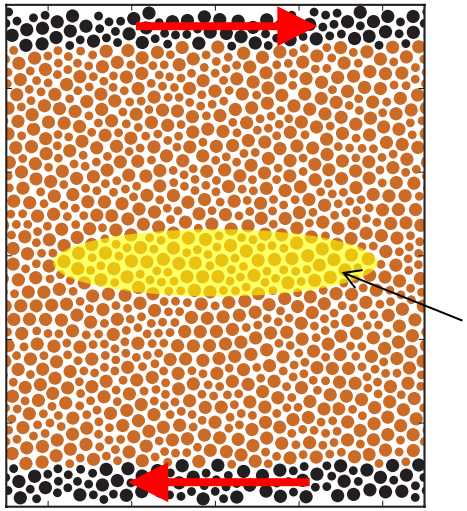
soft dendrites (ordered)

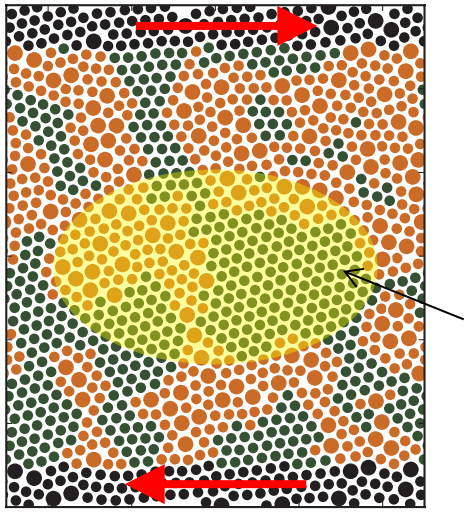




Which matters more - configurational or strength heterogeneity?

Why an Inhomogeneous Configuration Is More Ductile?





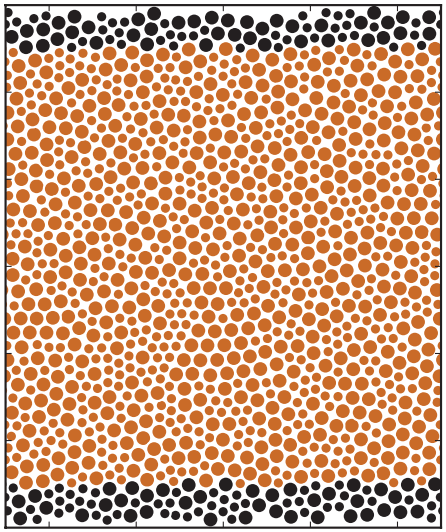
Idea:

An inhomogeneous configuration allows the system to deform more uniformly, which leads to reduced shear localization and therefore better ductility.

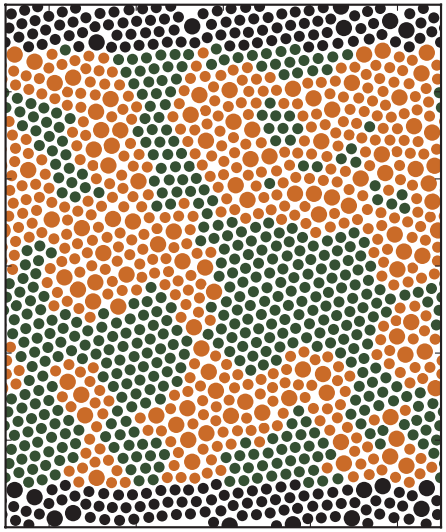
How to construct a mesoscopic inhomogeneous configuration?

A Disordered Bidisperse Mixture w/ a Disperse Ordered Phase

homogeneous



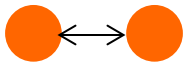
inhomogeneous



$N_{tot} = 1000, T = 0.2.$

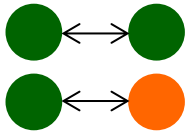
Inter-particle potentials:

stiff particles



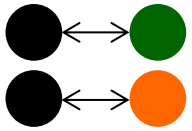
$V_{12\text{-}6}$

soft particles



$V_{8\text{-}6}$

boundary particles

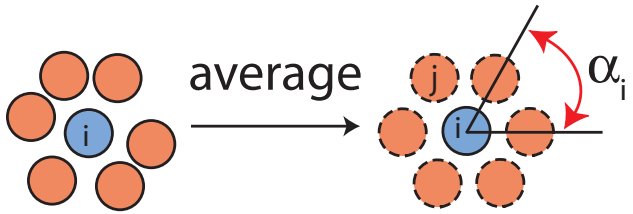


$V_{12\text{-}6}$

Area packing fraction $\varphi = 0.793$.

Modeling Tool (1)

A polycrystal model with a tunable crystallinity *(Onuki et al. 06', 07' 10')*

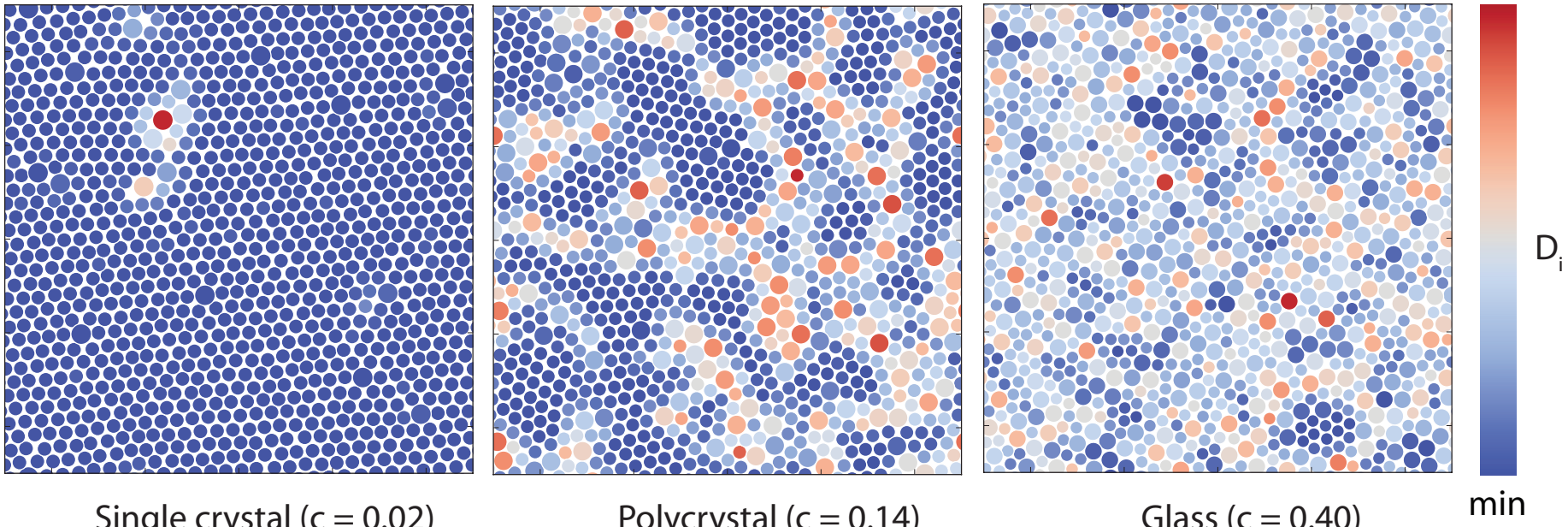


$$D_i = 2\Sigma_{j=\text{bonded}}[1-\cos 6(\alpha_i-\alpha_j)],\ 0<\alpha_i<\pi/3$$

α_i: particle crystalline angle

D_i: particle disorder variable

$C = N_L/N_{tot}$



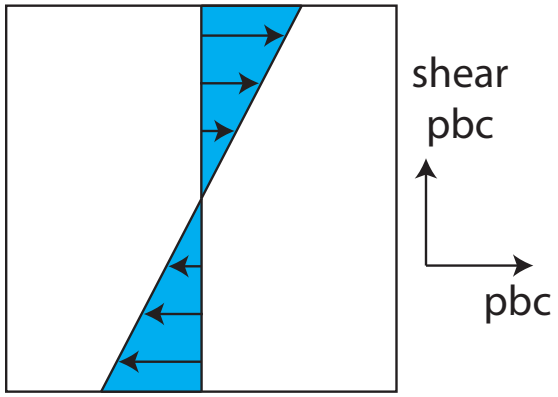
Single crystal (c = 0.02)

Polycrystal (c = 0.14)

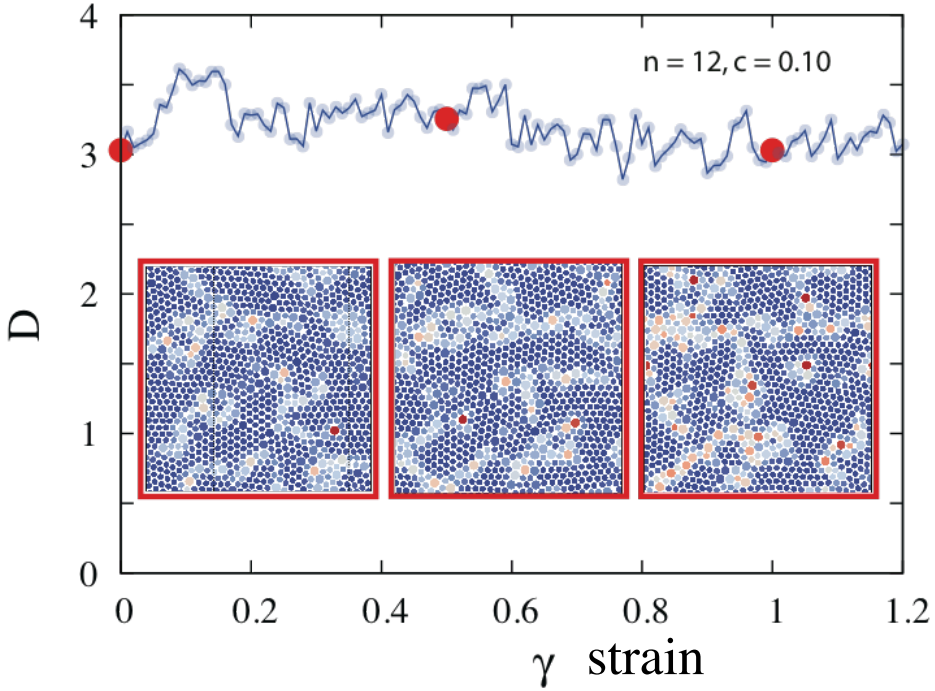
Glass (c = 0.40)

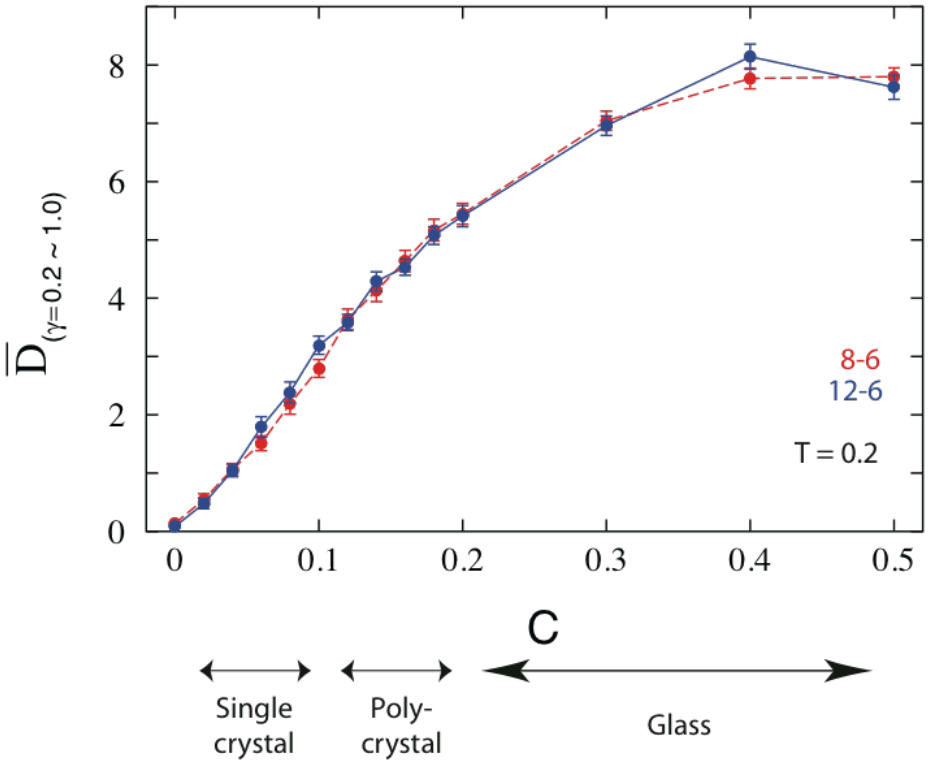
Persistent Crystallinity under Shear Deformation

NVT SLLOD algorithm



$d\gamma/dt = 10^{-4}$ (dimensionless)

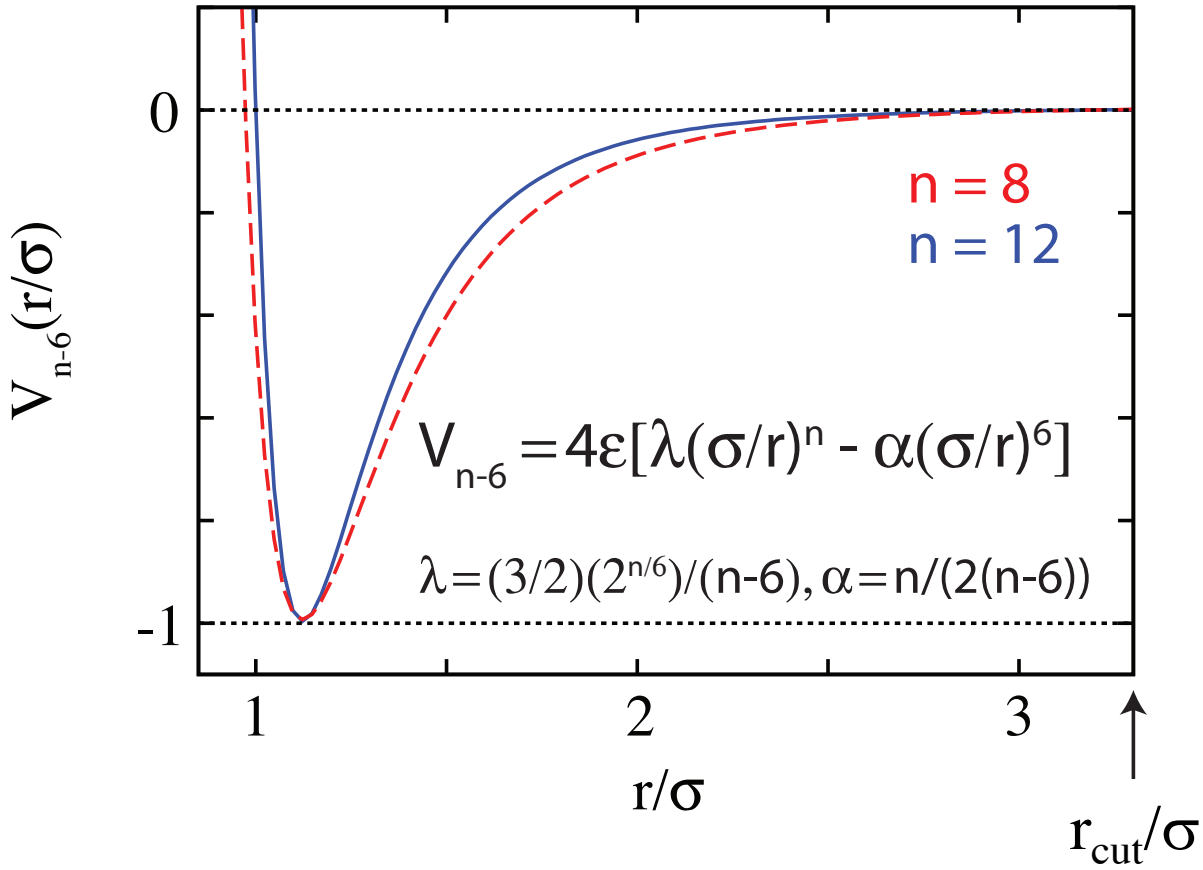




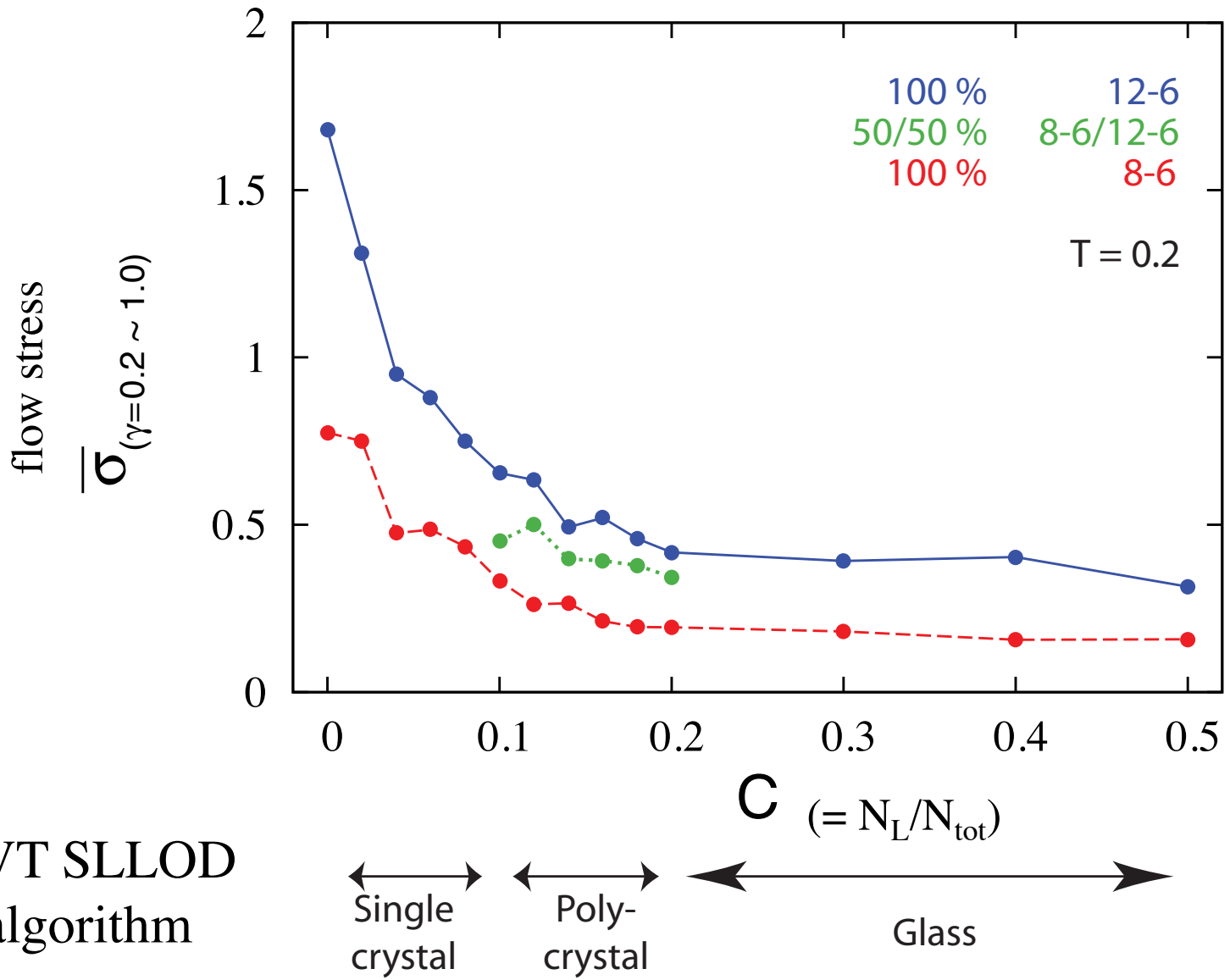
Modeling Tool (2)

Giving each phase different strength by using the n-6 Lennard-Jones potential

(P. Ginart et al. 11')



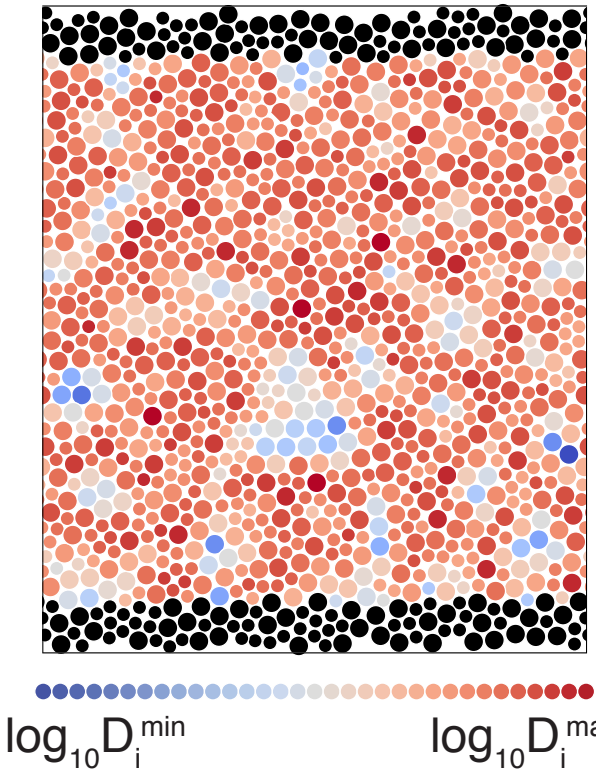
Tunable Mechanical Strength

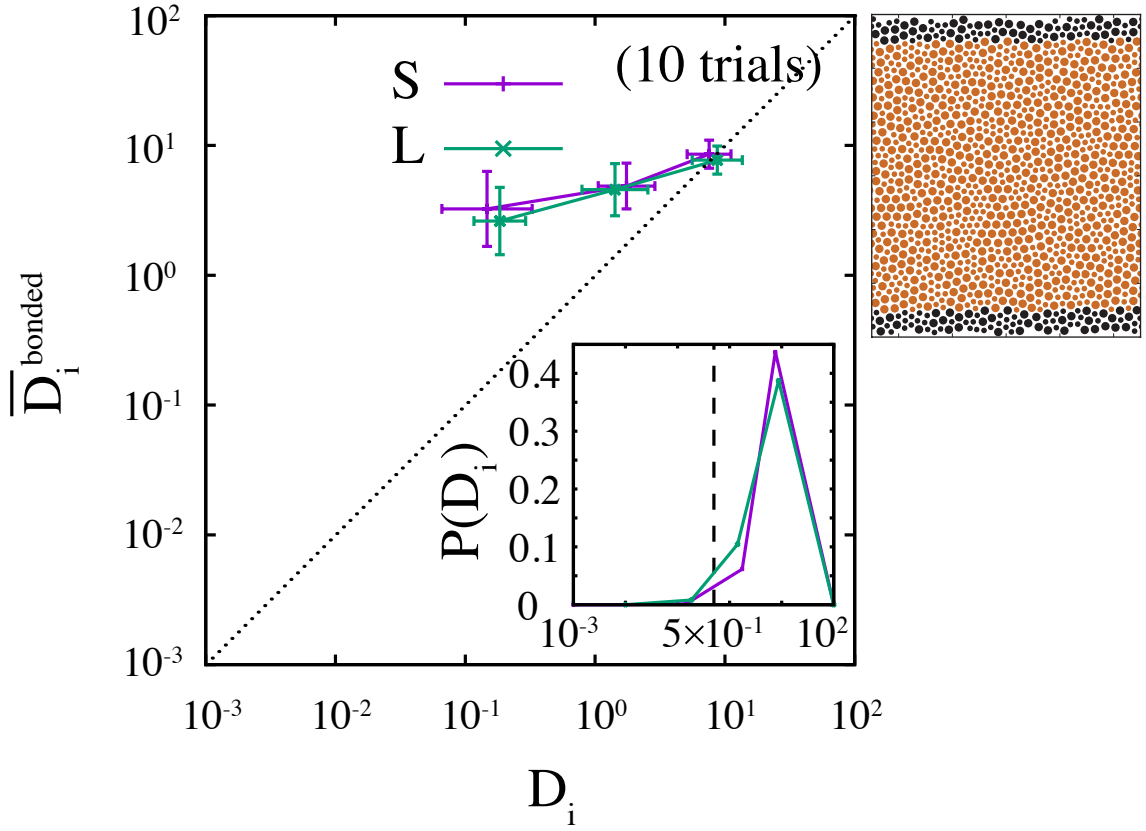


NVT SLLOD algorithm

How to Prepare a homogeneous Configuration?

$C = 0.5$, $N_{tot} = 1000$, $T = 0.2$

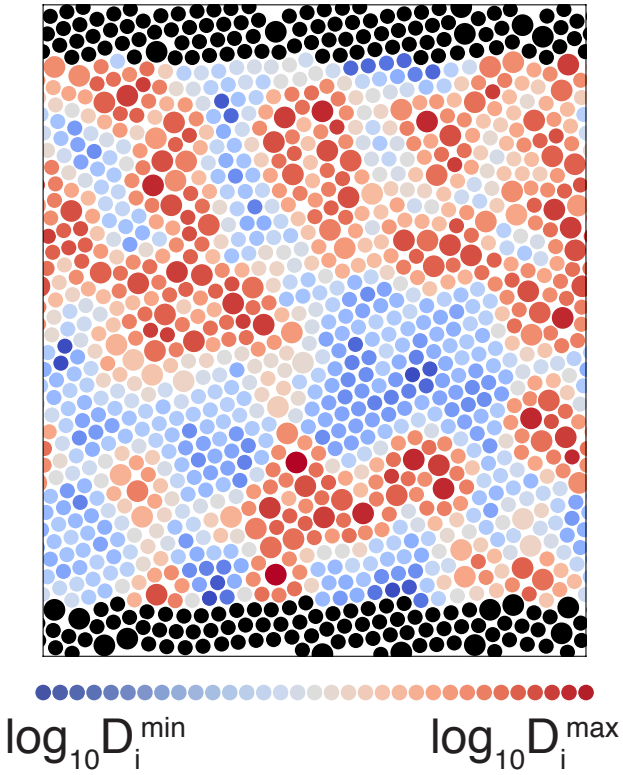


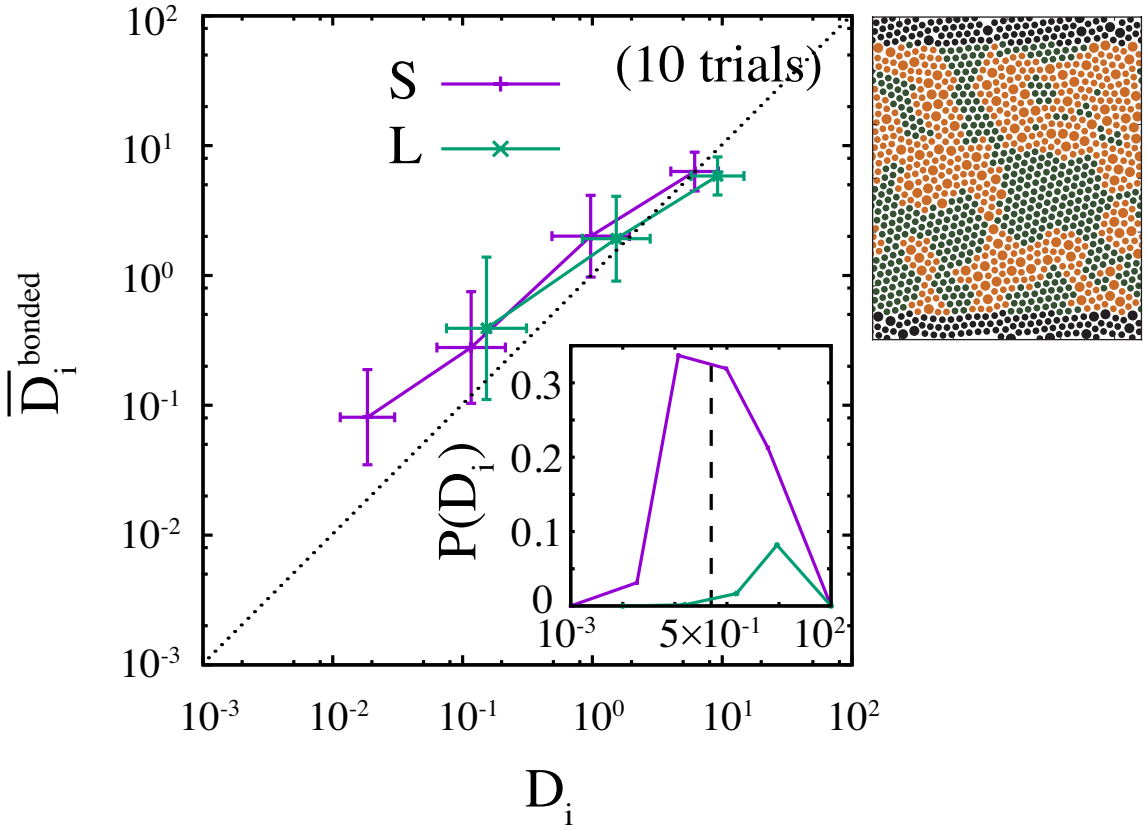


Most particles tend to have disordered neighbors.

How to Prepare an Inhomogeneous Configuration?

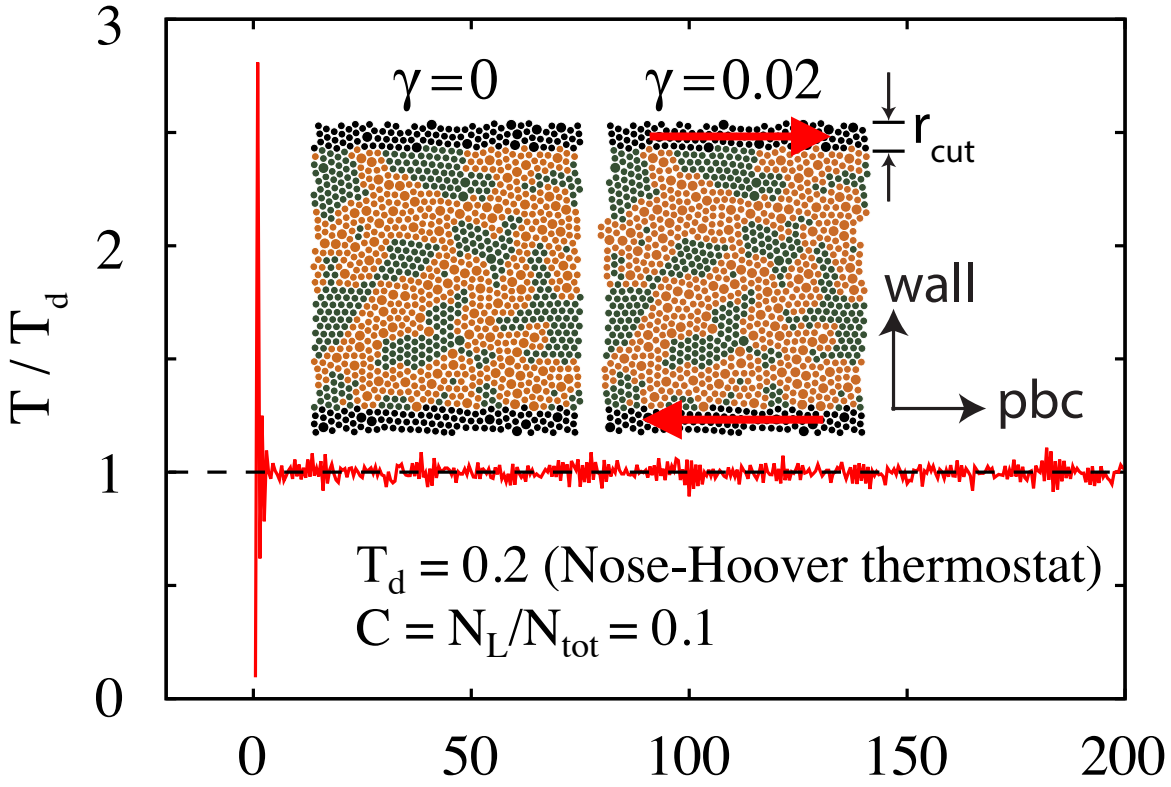
$C = 0.1$, $N_{tot} = 1000$, $T = 0.2$





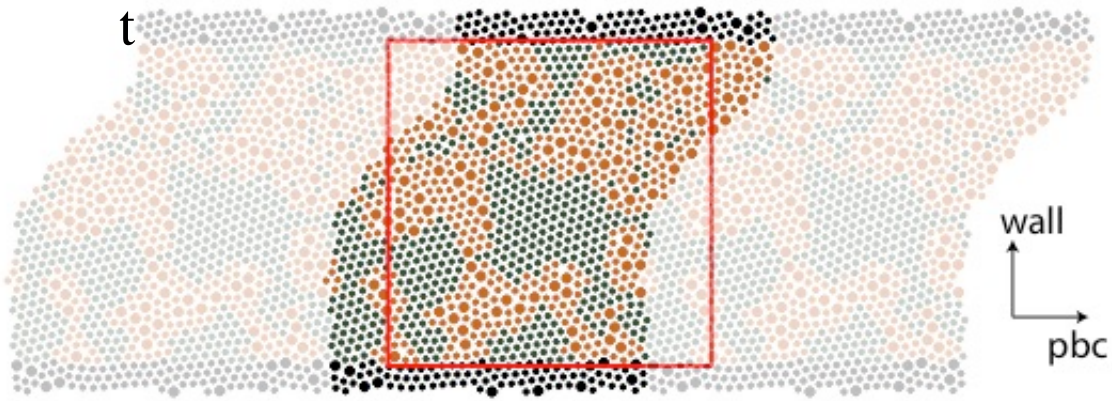
Ordered (disordered) particles tend to have ordered (disordered) neighbors.

Quasistatic Shear Deformation



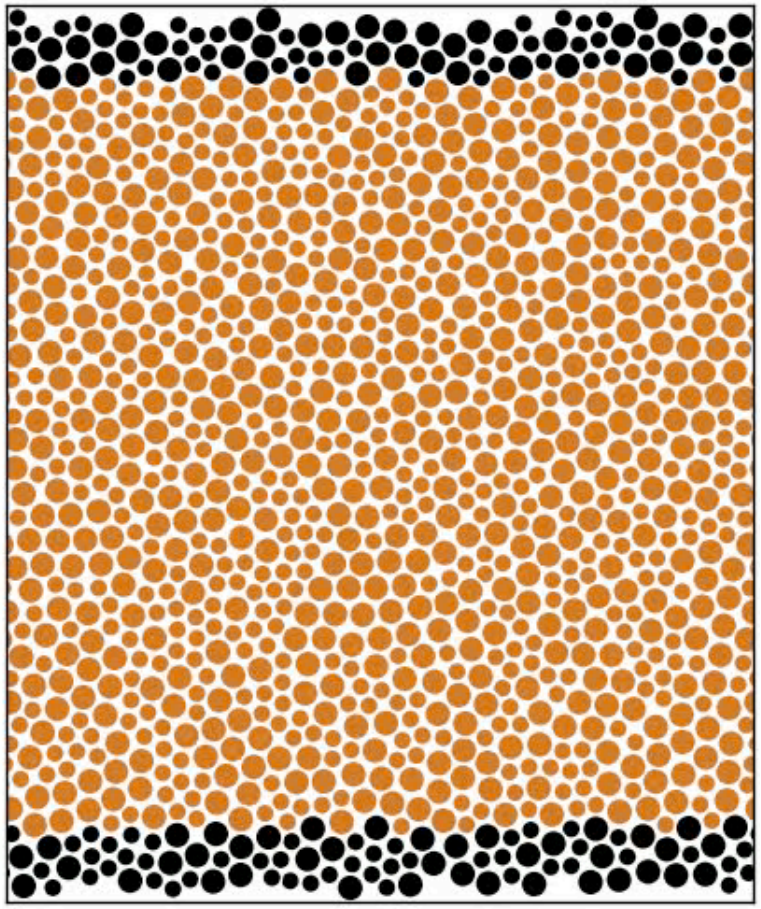
shear rate = 0.02/step

boundary conditions



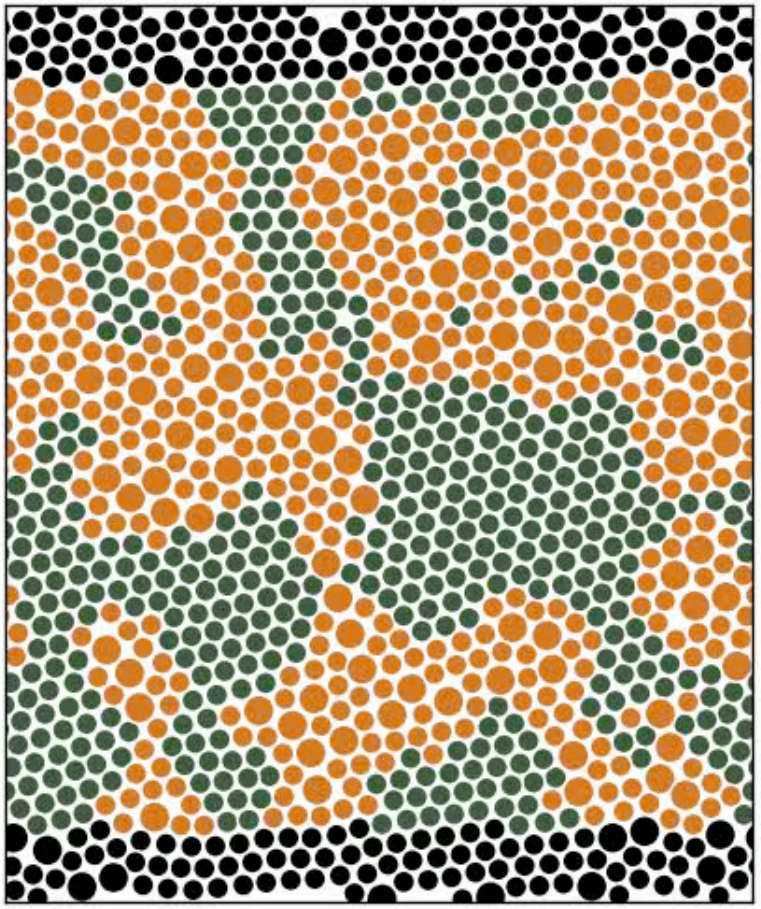
Quasistatic Shear Deformation

gamma (strain) = 0.02



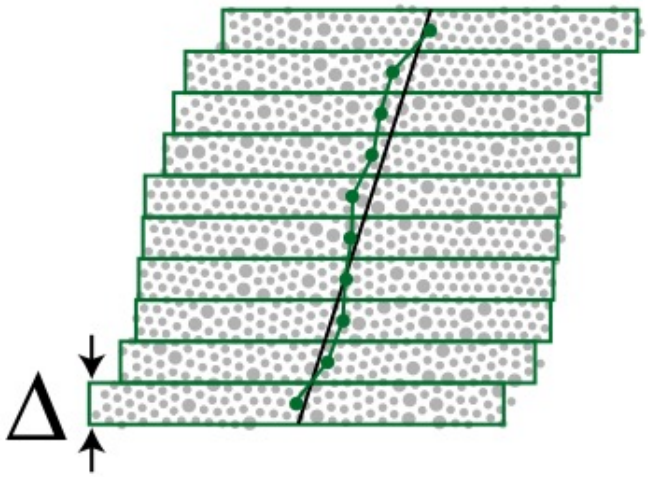
homogeneous

gamma (strain) = 0.02



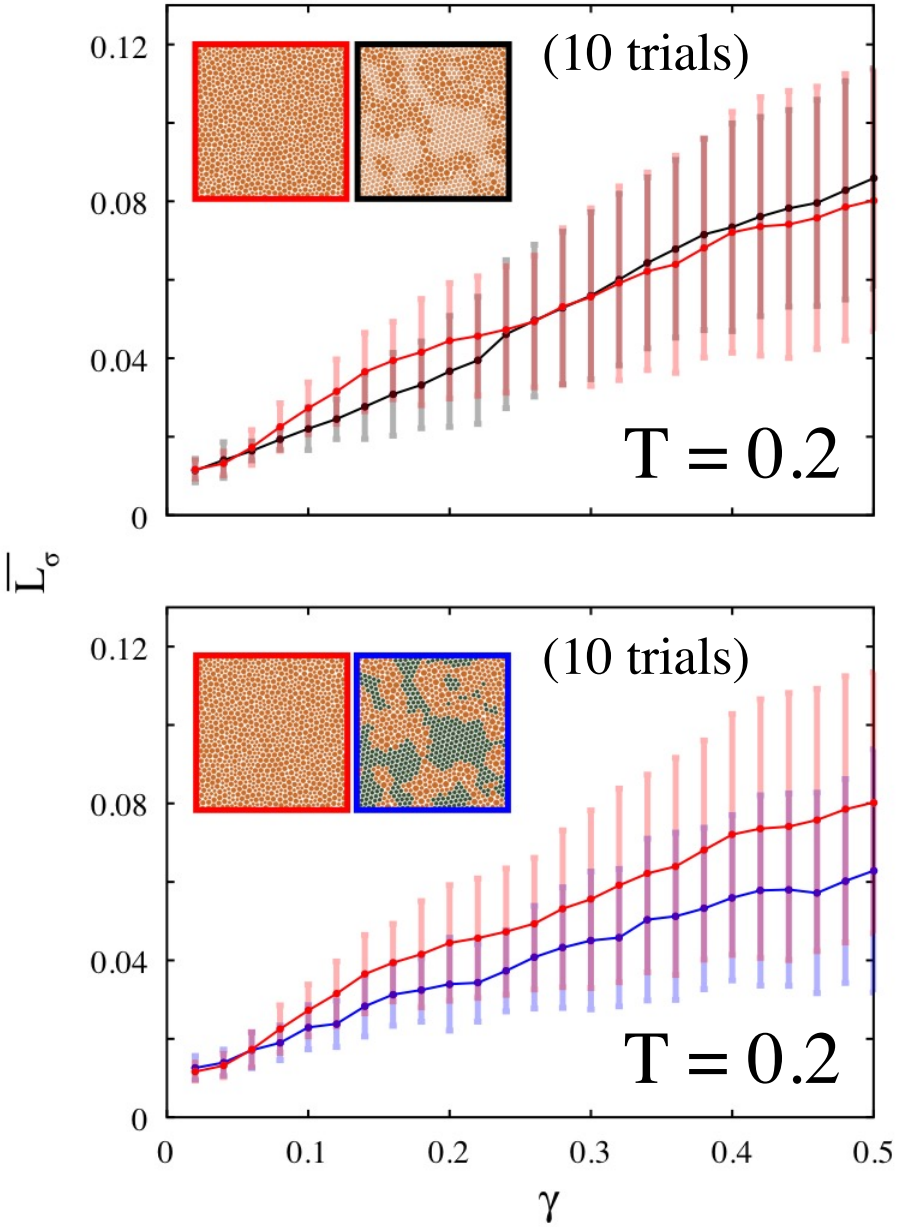
inhomogeneous

An Inhomogeneous Configuration Deforms Most Uniformly

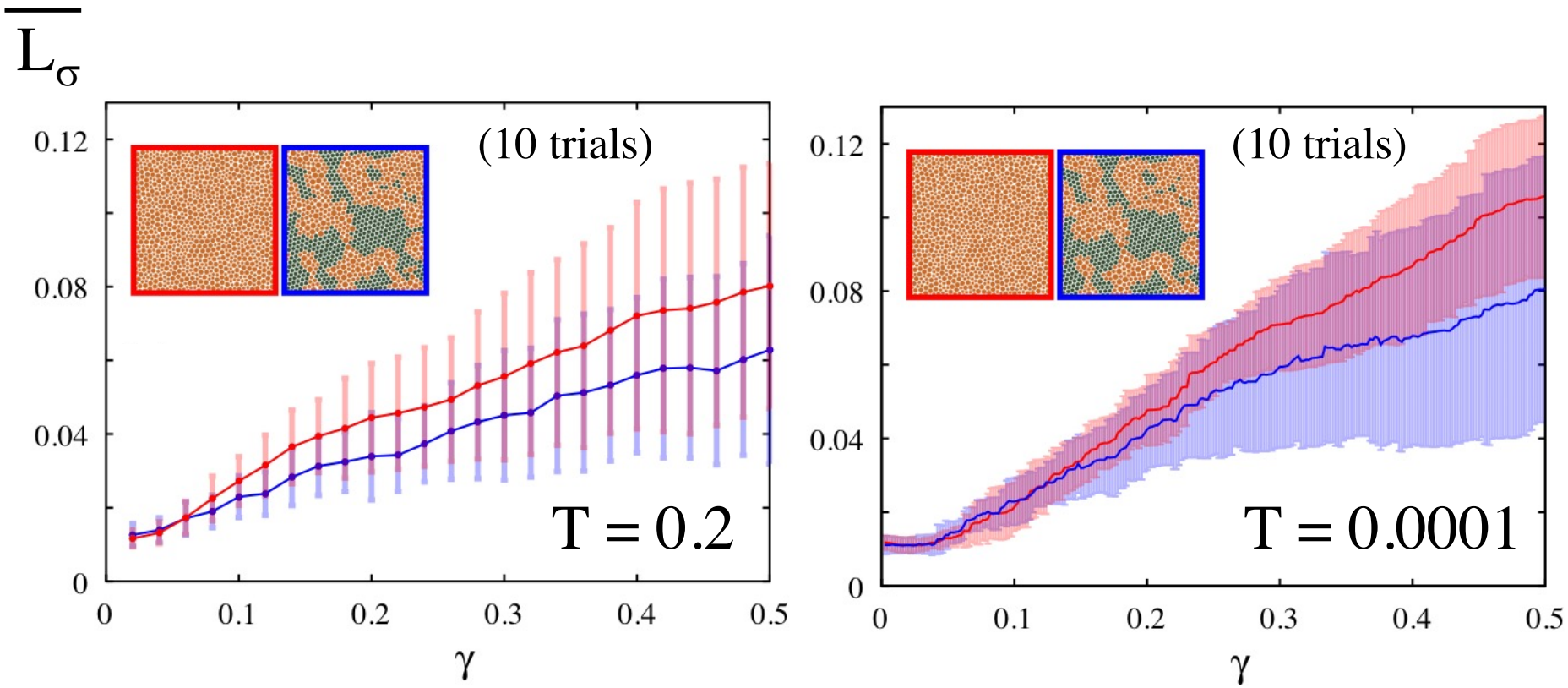


L_σ: deviation from the affined deformation.

$\Delta = L_y/10$



Verifying the Trend at Near-Zero Temperature



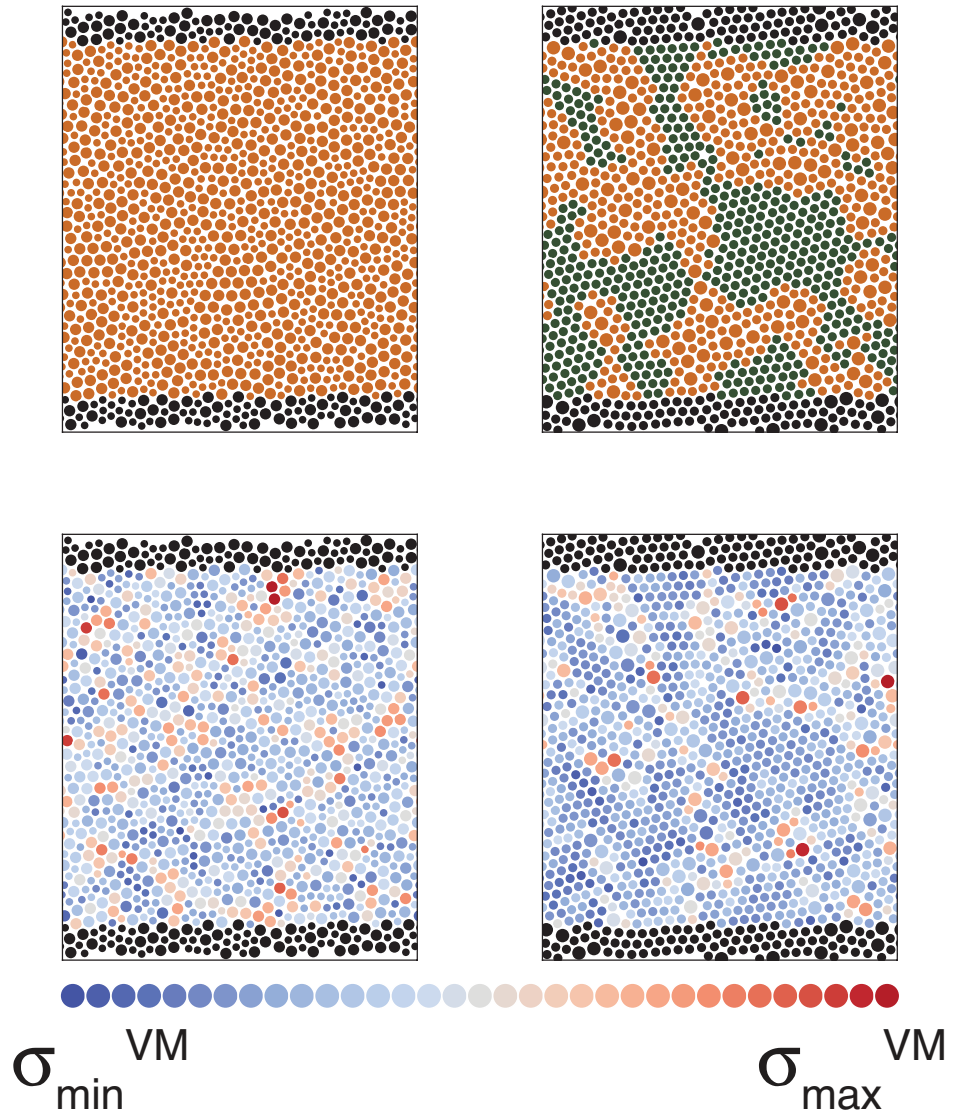
shear rate = 0.02/step

shear rate = 0.002/step

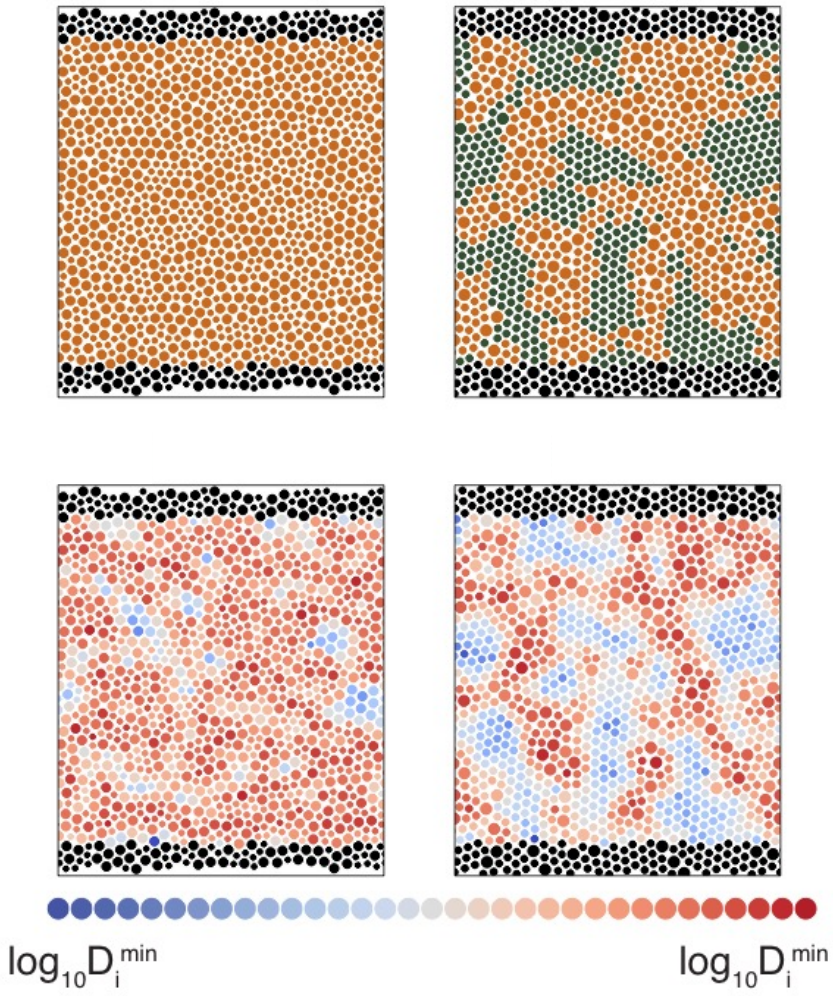
Increasing number of trials does not change the trend.

Why an Inhomogeneous Configuration Deforms More Uniformly?

Von Mises shear stress

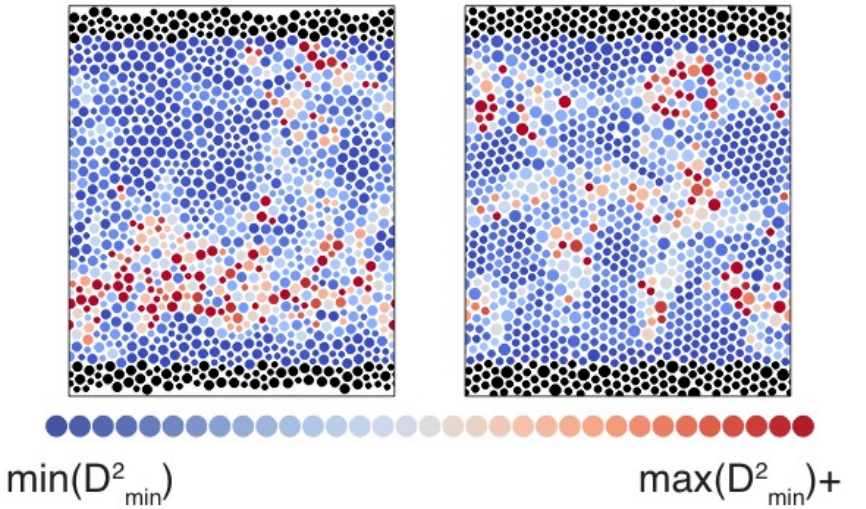


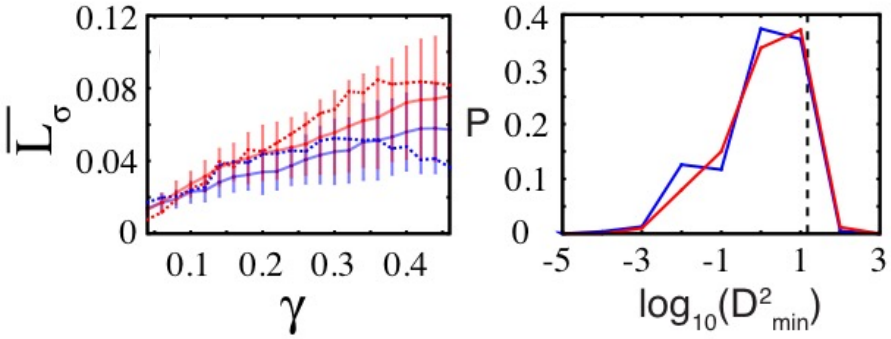
Why an Inhomogeneous Configuration Deforms More Uniformly?



γ = 0.46

(reference: γ = 0.04)





D^2_{min}: local irreversible shear deformations

Summary and Future Work

- We propose a disordered bidisperse mixture having:
  1) a disperse ordered phase;
  2) different strengths between different phases.

- Our mesoscopic model qualitatively shows that an inhomogeneous composition deforms more uniformly than a homogeneous one, which presumably leads to weaker shear localization/banding and therefore improves the ductility.

- Examining a hard ordered phase embedded in a soft disordered matrix and exploring the optimal ordered/disordered area ratio that gives the best deformation uniformity.

Acknowledgement

Startup funding, Shizuoka University, Japan.