Controlled mechanical response in glasses via designed spatial inhomogeneity

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Statphys Meeting ICTS
February 1-3, 2023

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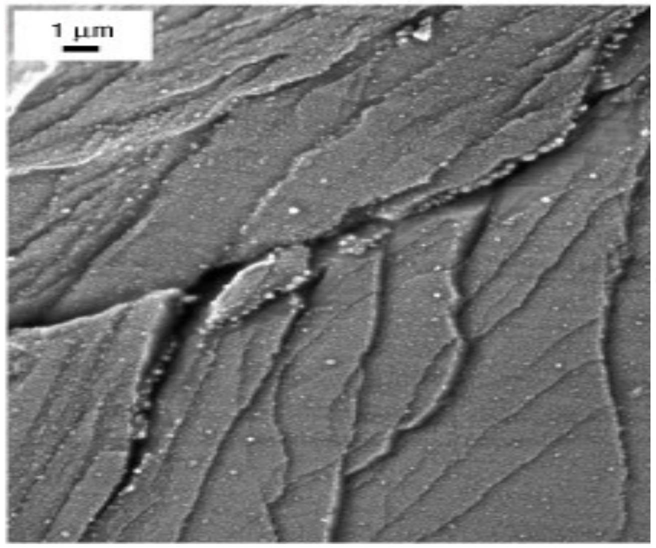
Jürgen Horbach, HHU Düsseldorf

Deformed amorphous solids: inhomogeneous patterns

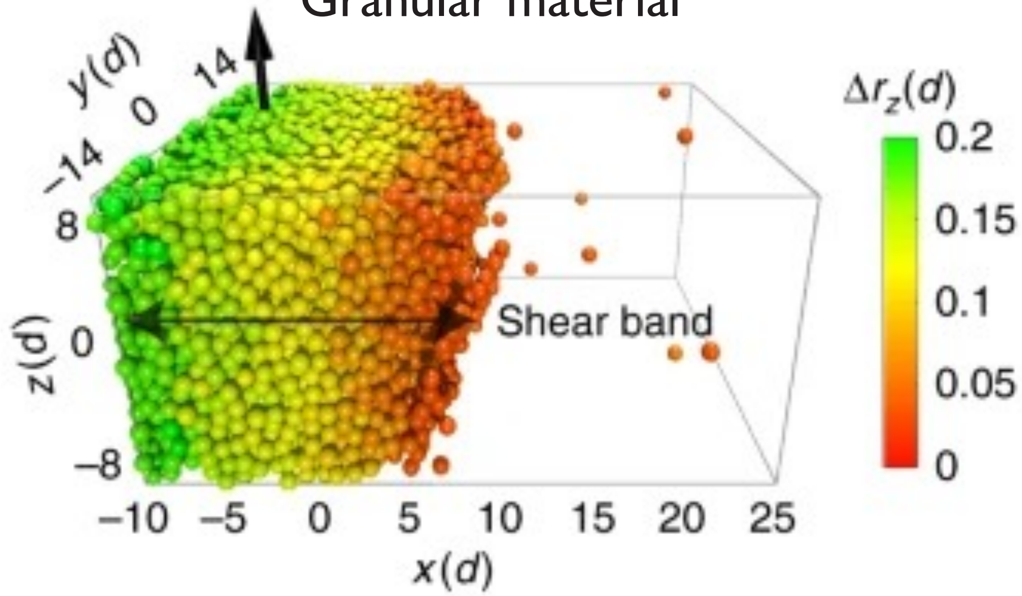
Experiments

Metallic glass



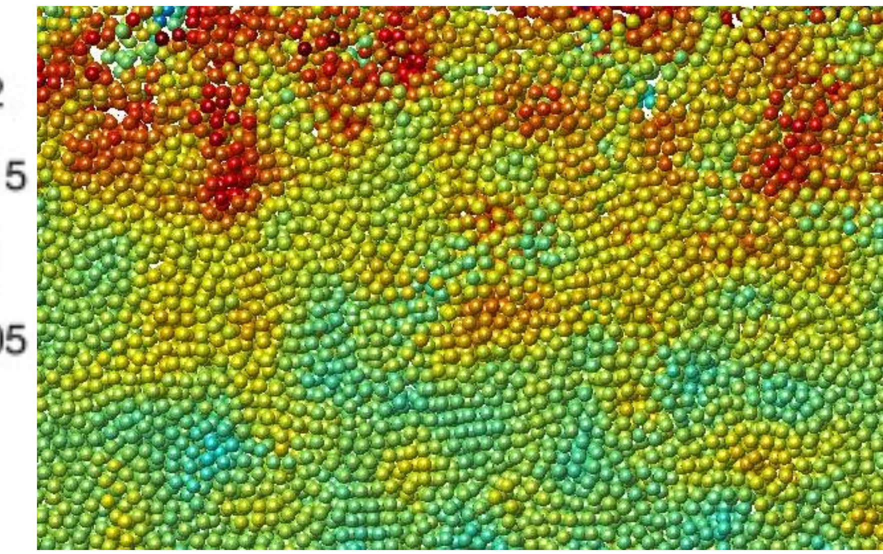
J. J. Lewandowski et al.
Nat. Mat. 5, 15 (2006)

Granular material



Y. Cao et al.
Nat. Comm. 9, 2911 (2018)

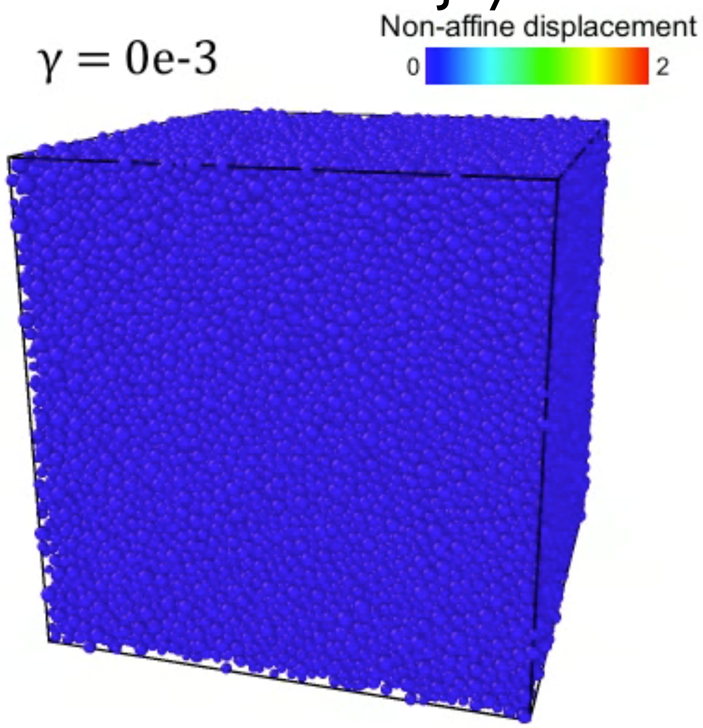
Colloidal glass



V. Chikkadi et al.
PRL 107, 198303 (2011)

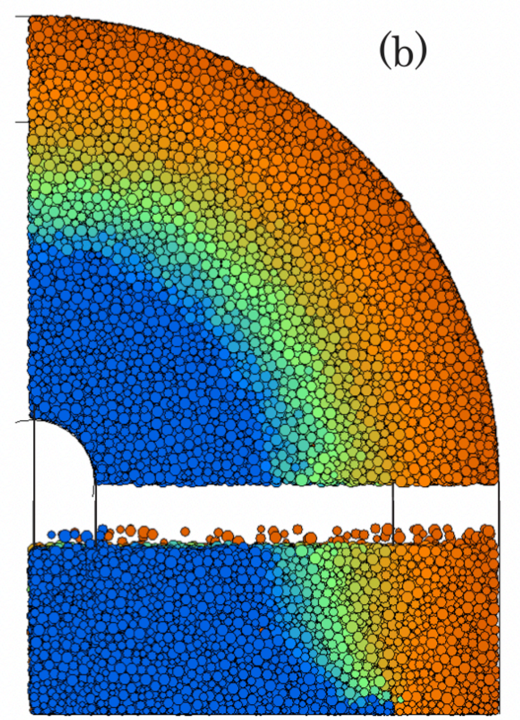
Computer Simulations

MD simulation: LJ system



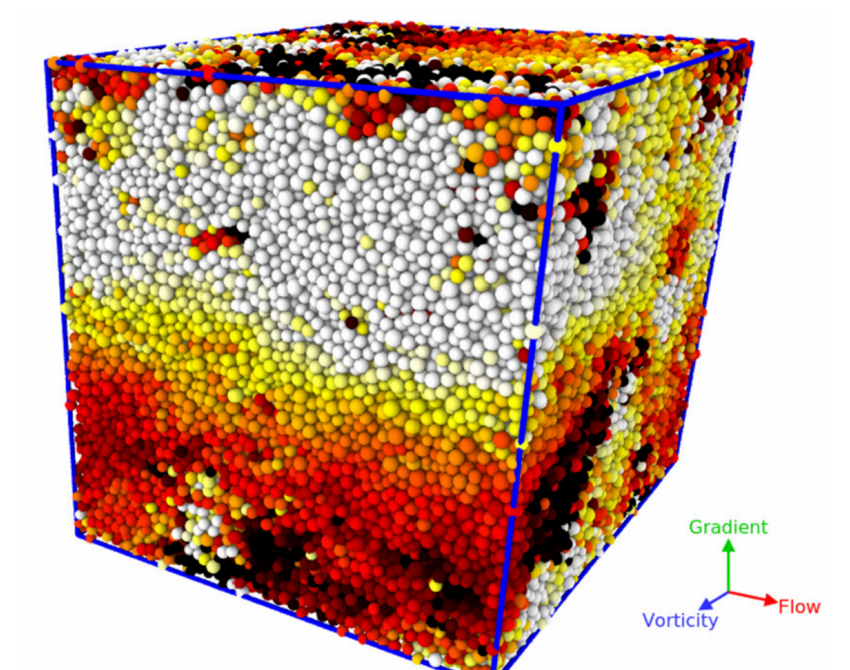
M. Ozawa et al.
PNAS 115, 26 (2018)

DEM simulation: granular powder



A. Singh et al.
PRE 90, 22202 (2014)

MD simulation: soft repulsive suspension



V.Vasisht et al.
PRE 102, 12603 (2020)

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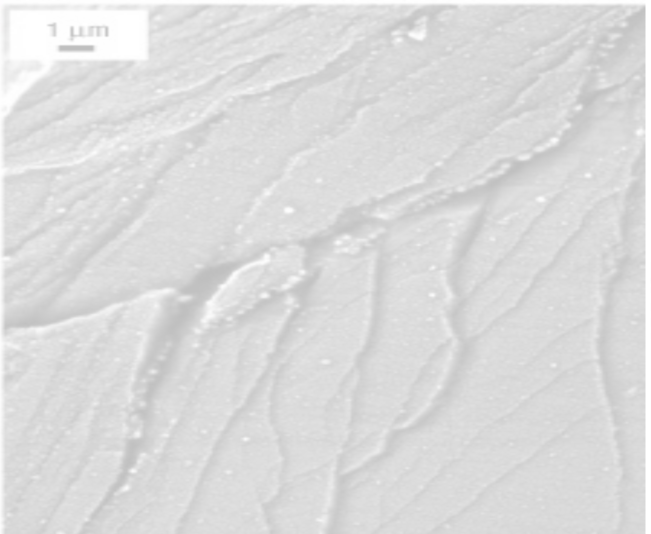

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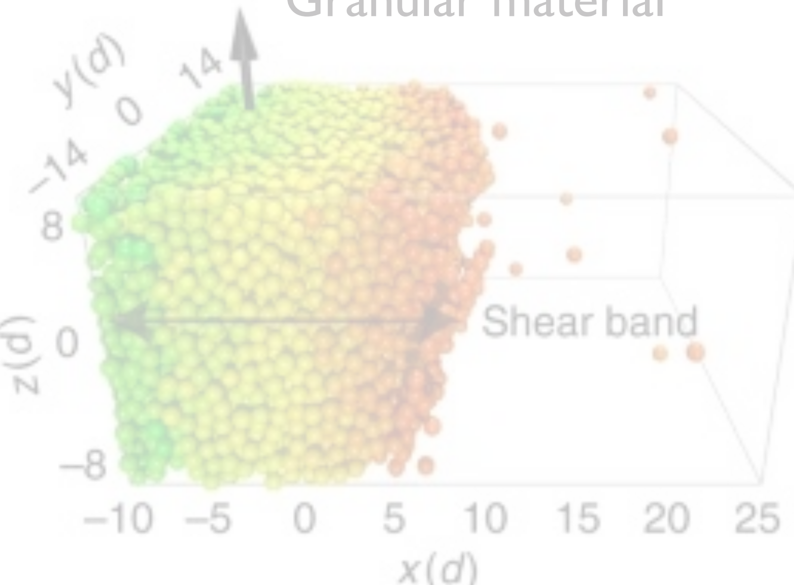

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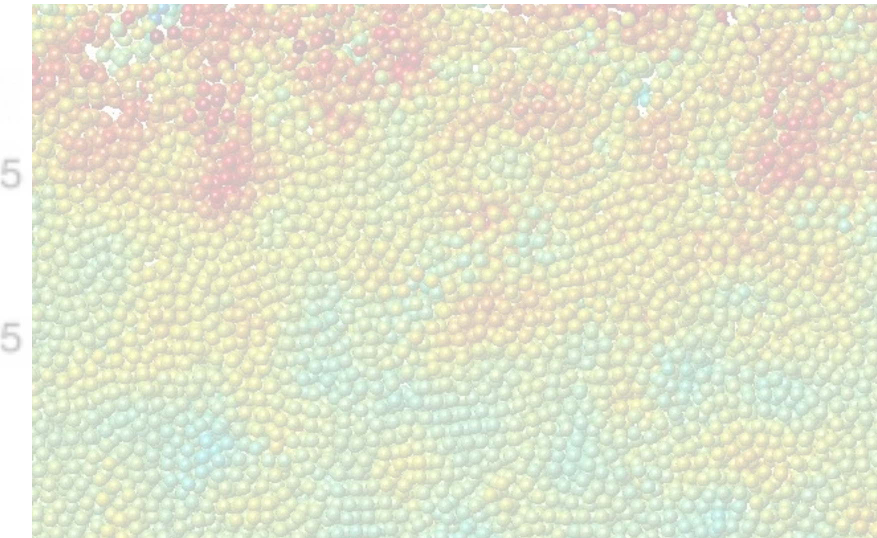

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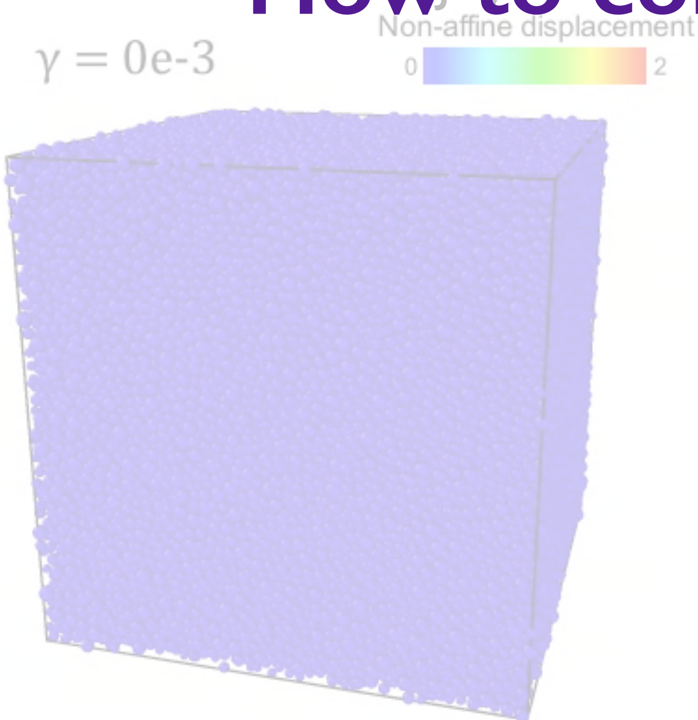
Shear band nucleation is stochastic?

How to control the nucleation and growth?

Computer Simulations



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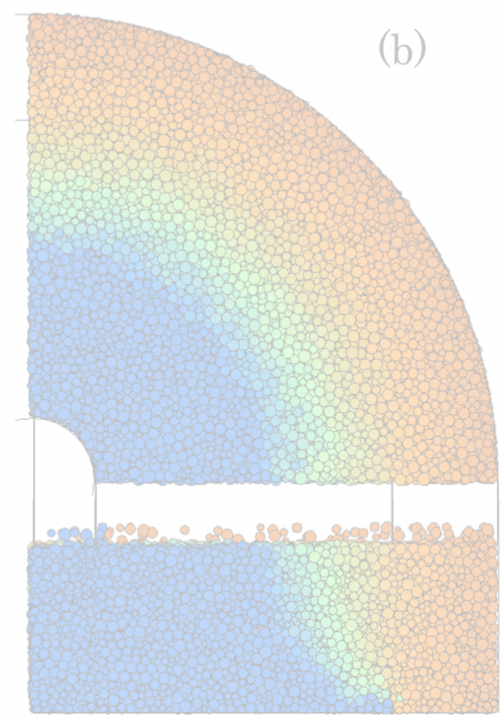

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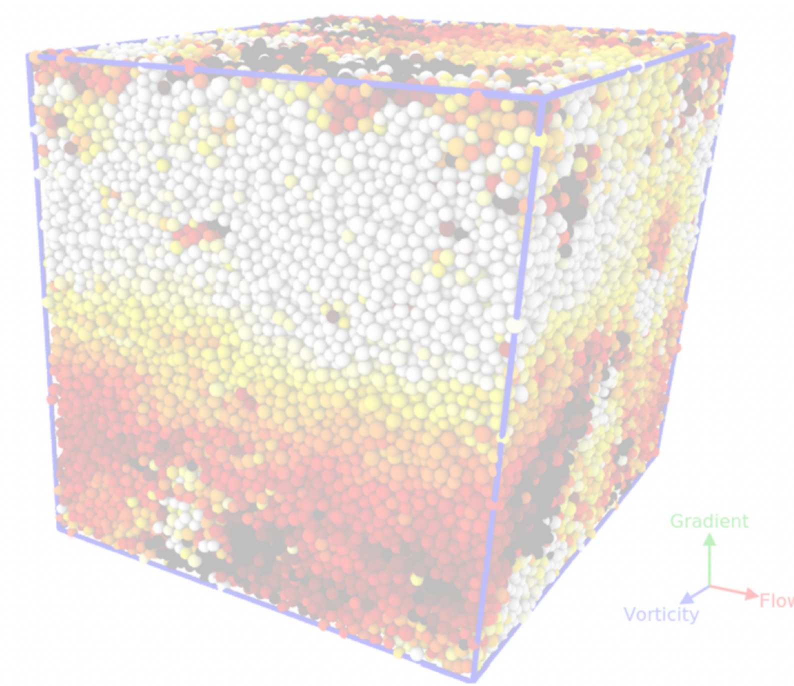
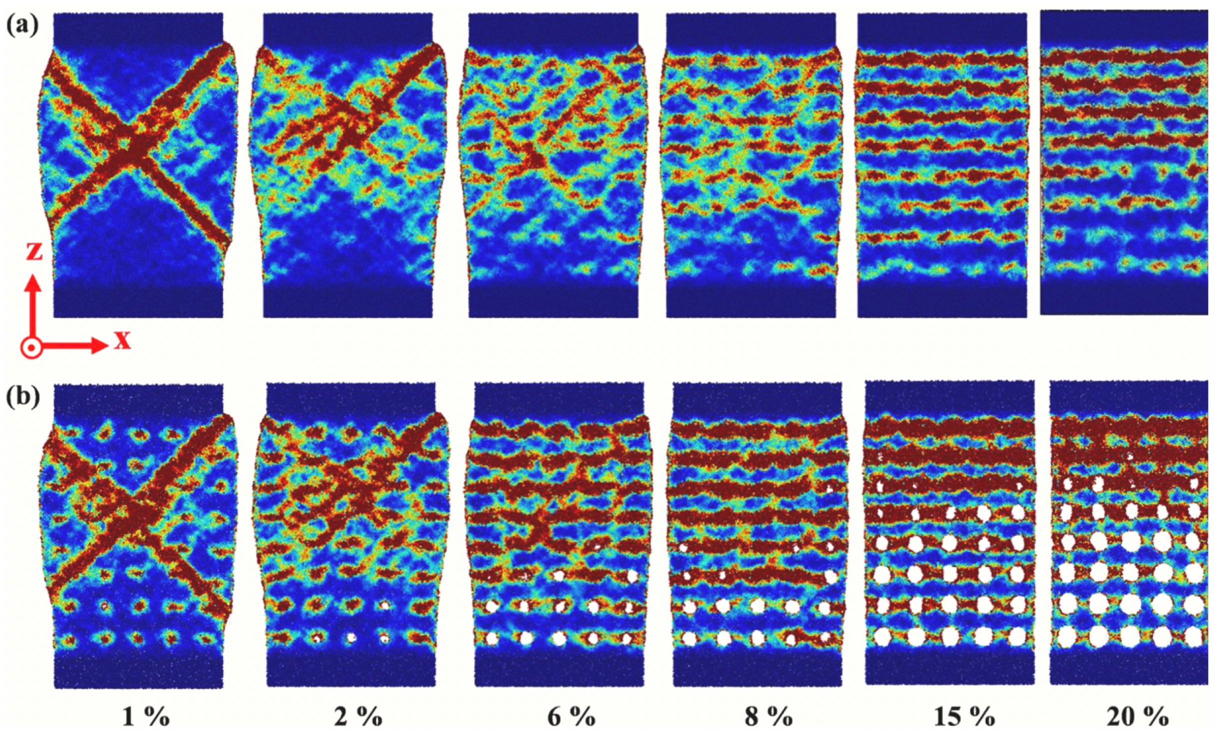
repulsive suspension



V. Vasisht et al.
PRE 102, 12603 (2020)

Controlling the shear band nucleation and growth



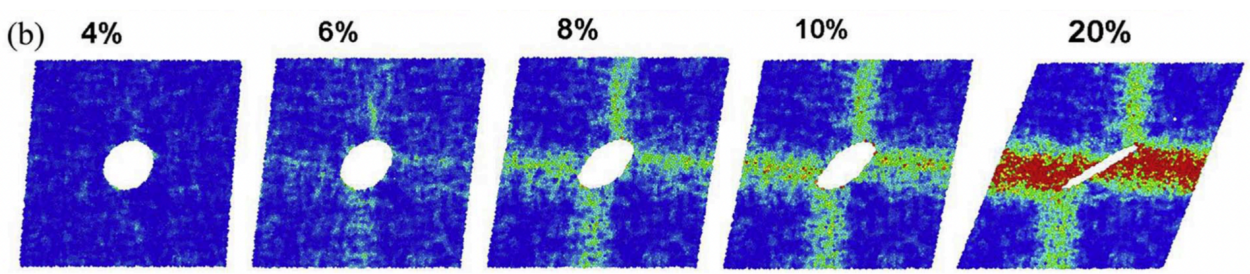
Control of shear band formation in metallic glasses through introducing nanoscale pores

X.Q. Lu [a], L. Li [b], Y.H. Zhang [a], Z.J. Li [a], S.D. Feng [a,*], L.M. Wang [a,*], R.P. Liu [a]

[a] *State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China*
[b] *Department of Metallurgical and Materials Engineering, The University of Alabama, Tuscaloosa, AL 35487, USA*

Deformation of Porous glass

Control over: yield strength, elastic modulus, direction band propagation

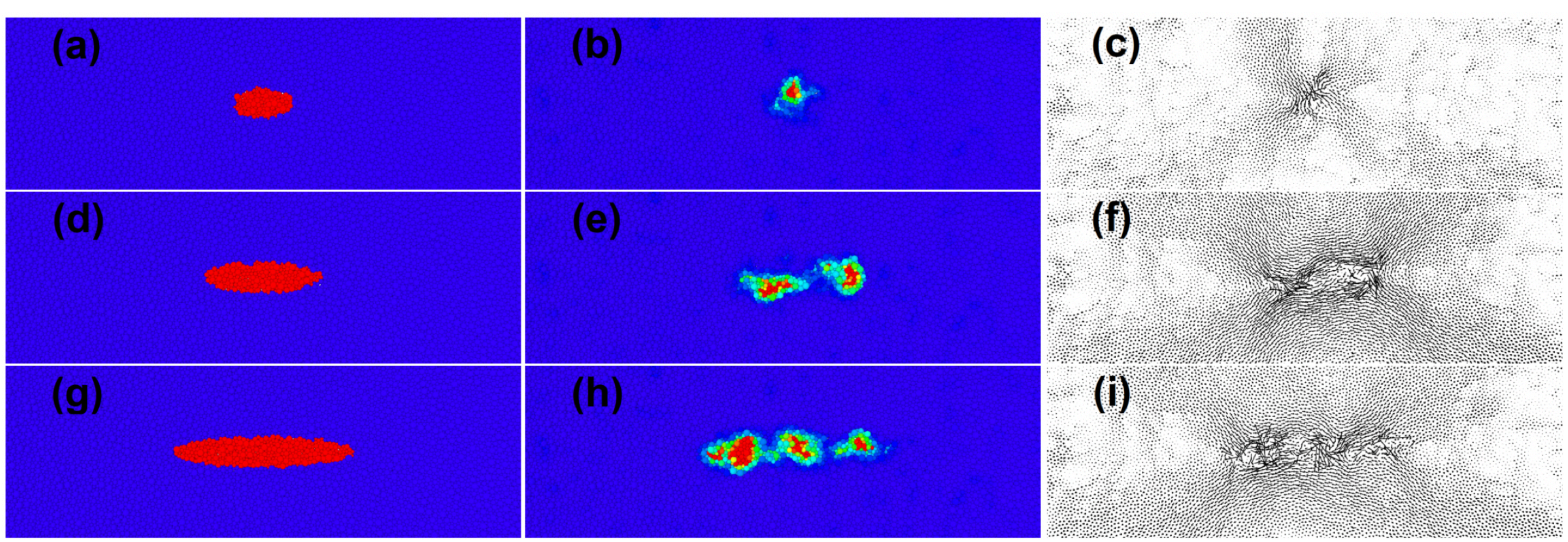


Early nucleation; near voids

The effect of void defects on the shear band nucleation of metallic glasses

Yun Luo[a,b], Guannan Yang[a,b,*], Yang Shao[a,b], Kefu Yao[a,b,**]

[a] *School of Material Science and Engineering, Tsinghua University, Beijing, 100084, PR China*
[b] *Key Laboratory for Advanced Materials Processing Technology, Ministry of Education, Beijing, 100084, PR China*



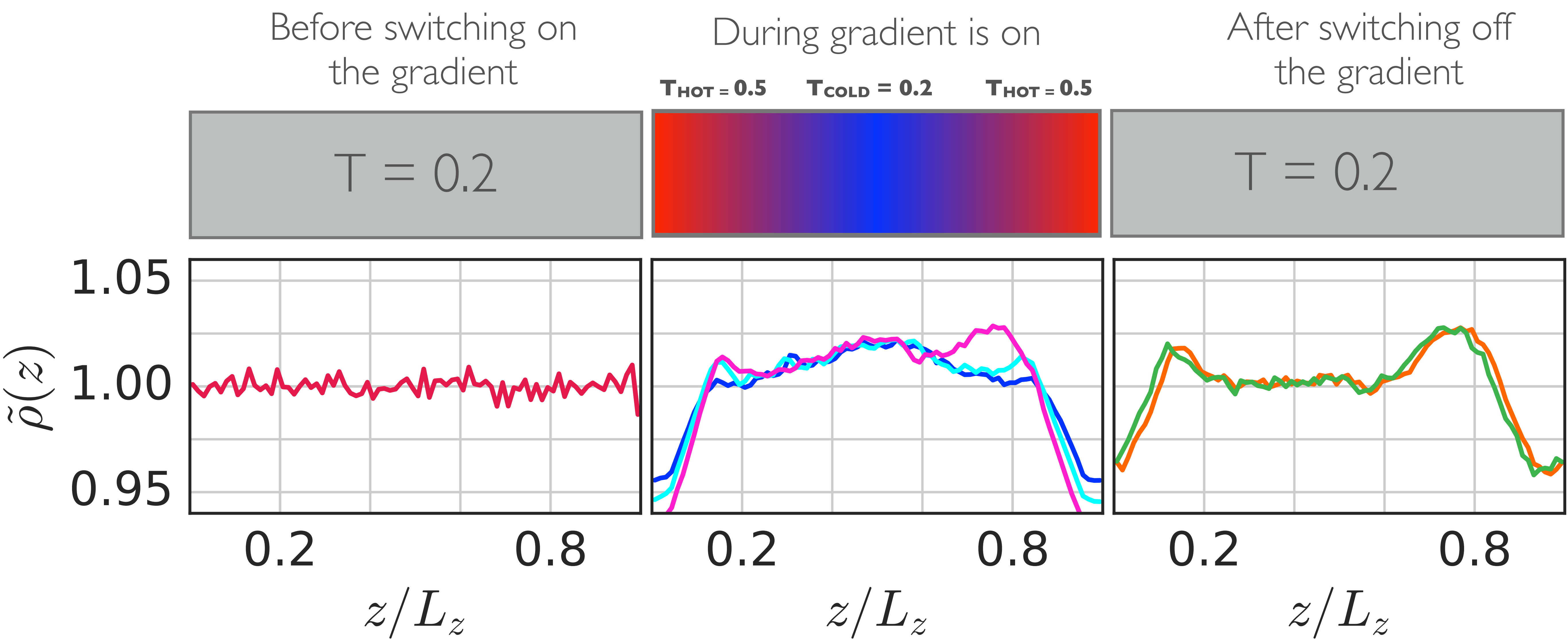
Synthetic soft region in well-annealed glass

Shear band nucleation in soft regions

Ozawa, Berthier, Biroli, and Tarjus, PRR, **4**, 23227602 (2022)

Designing Spatially Inhomogeneous Glasses

MD simulation of model binary LJ glass-former: $T_{MCT} \sim 0.435$, $T_g \sim 0.3$
Apply a temperature gradient pulse



Inhomogeneous structures are stable over a longer period of time

V. Vaibhav, J. Horbach and P. Chaudhuri; Phys. Rev. E 101, 022605 (2020)

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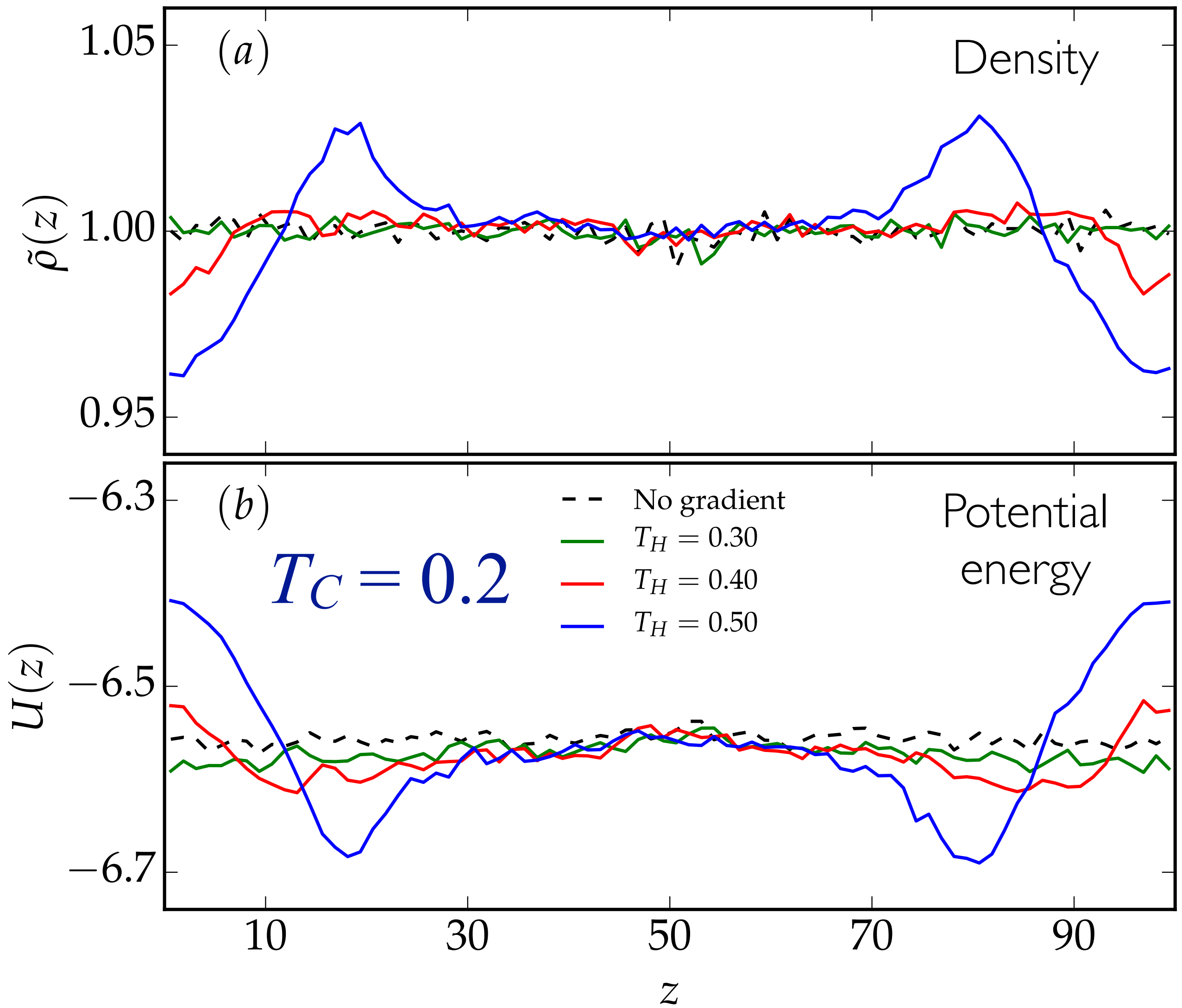
Designing Spatially Inhomogeneous Glasses

Varying gradient strength, fixed exposure time

Profiles after switching off the gradient



Order of heterogeneity depends on
— size of thermal gradient
— exposure time of thermal gradient

Nature of heterogeneity depends on T_H
— Rejuvenation vs melting

$T_{MCT} \sim 0.435$, $T_g \sim 0.3$

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Varying gradient strength, fixed exposure time

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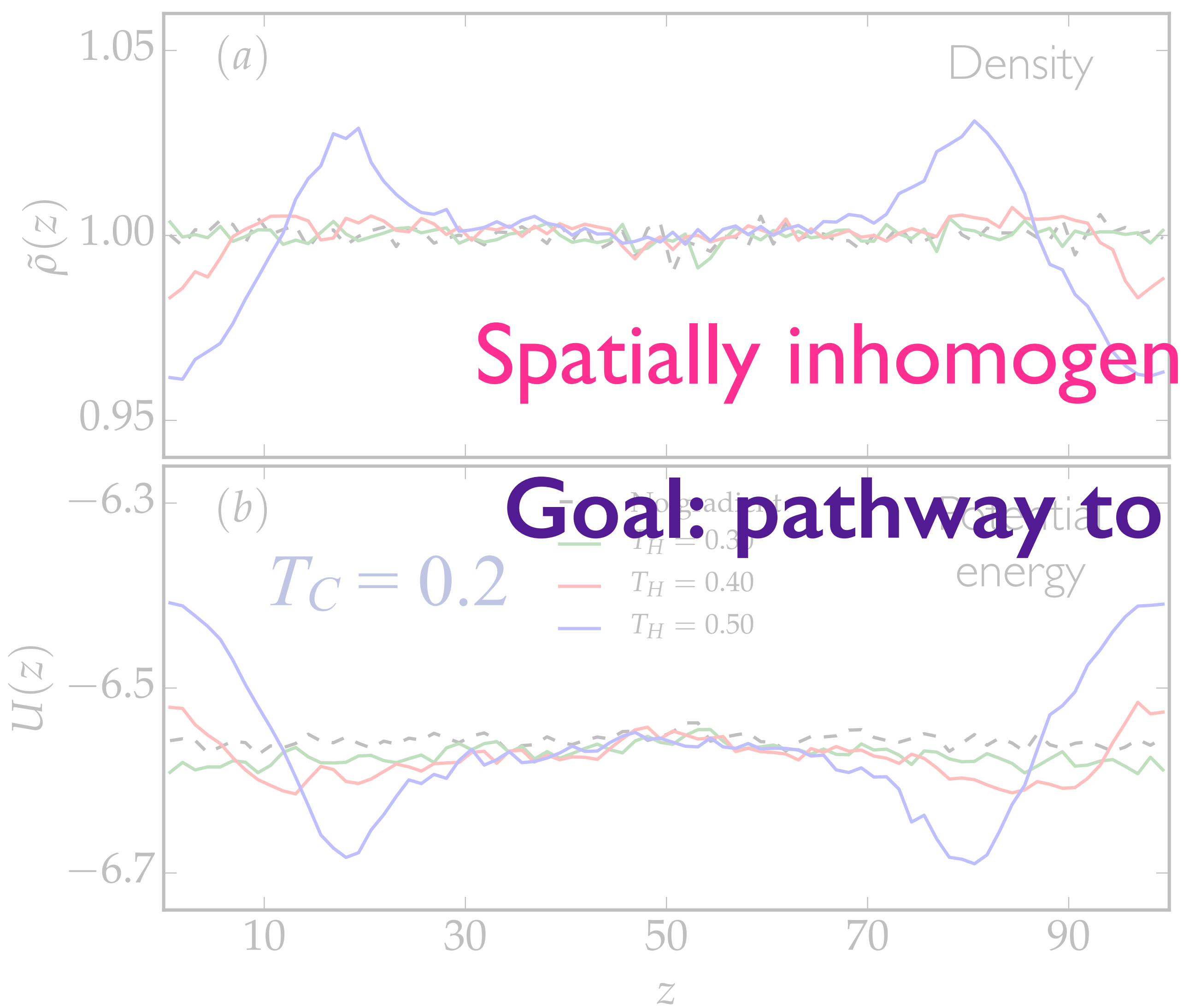


Spatially inhomogeneous glass at T = 0.2

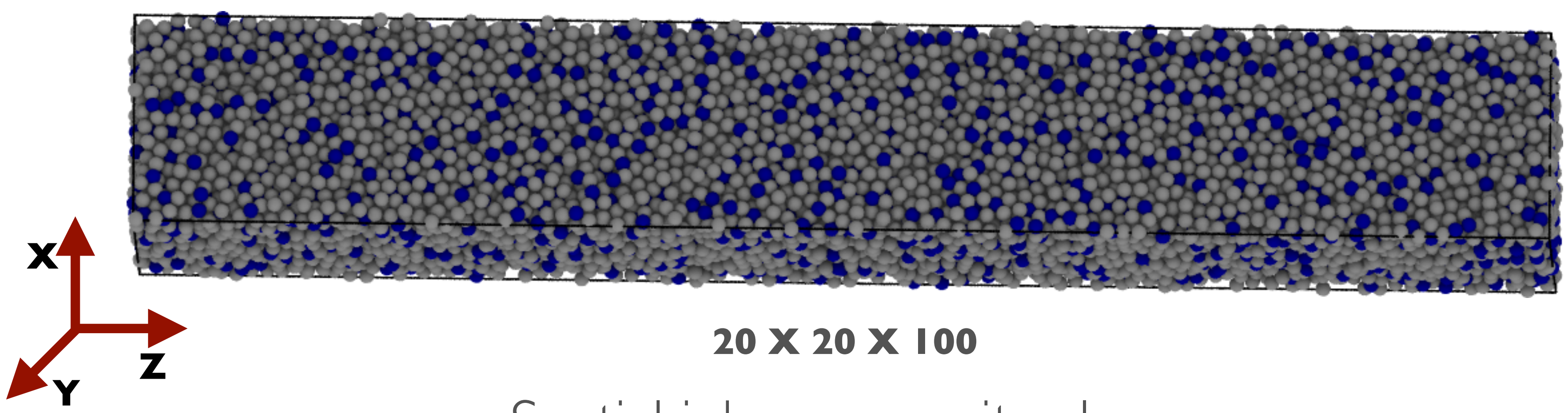
Goal: pathway to mechanical failure

Order of heterogeneity depends on
— size of thermal gradient
— exposure time of thermal gradient

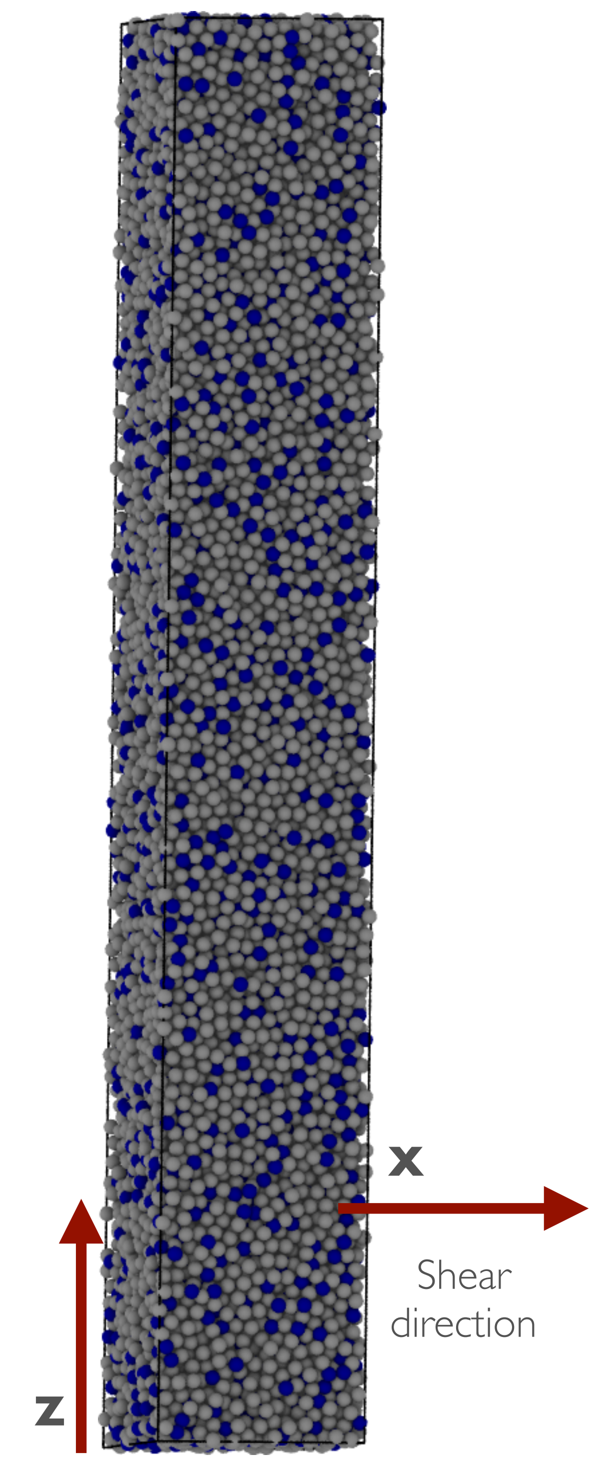
Nature of heterogeneity depends on T_H
— Rejuvenation vs melting

$T_{MCT} \sim 0.435$, $T_g \sim 0.3$

Shear response of thermally processed states



Spatial inhomogeneity along
Z-direction



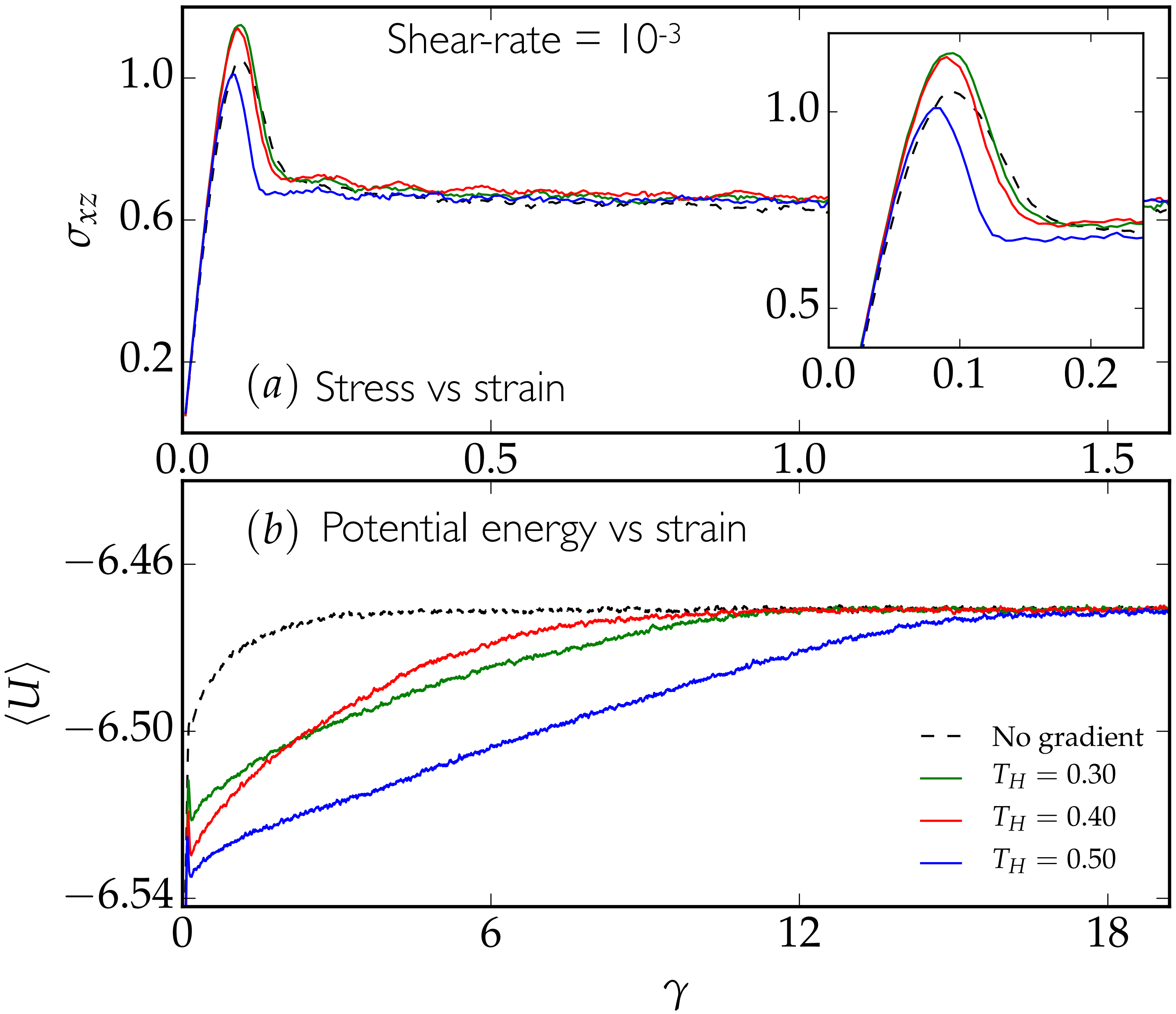
Deforming the heterogeneous samples at fixed shear-rates

XZ-plane is sheared along X-direction

T = 0.2 maintained using DPD thermostat

Shear response of thermally processed states

Deforming the heterogeneous samples at fixed shear-rates at fixed temperature (T = 0.2)



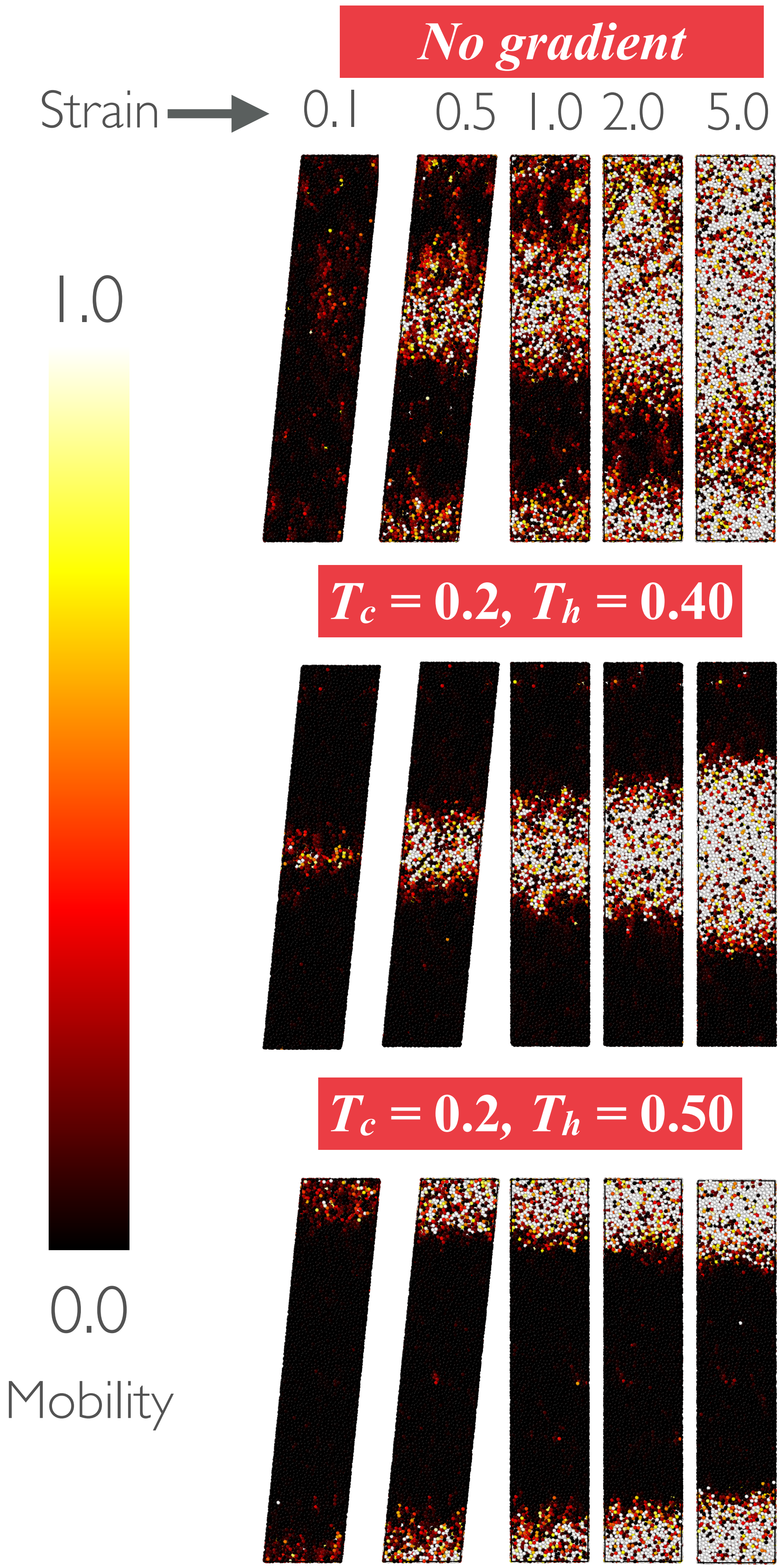
$T_C = 0.2$

$T_H = 0.30, 0.40, 0.50$

Modified yielding response

#Timescale for emergence of non-equilibrium steady-state depends on history

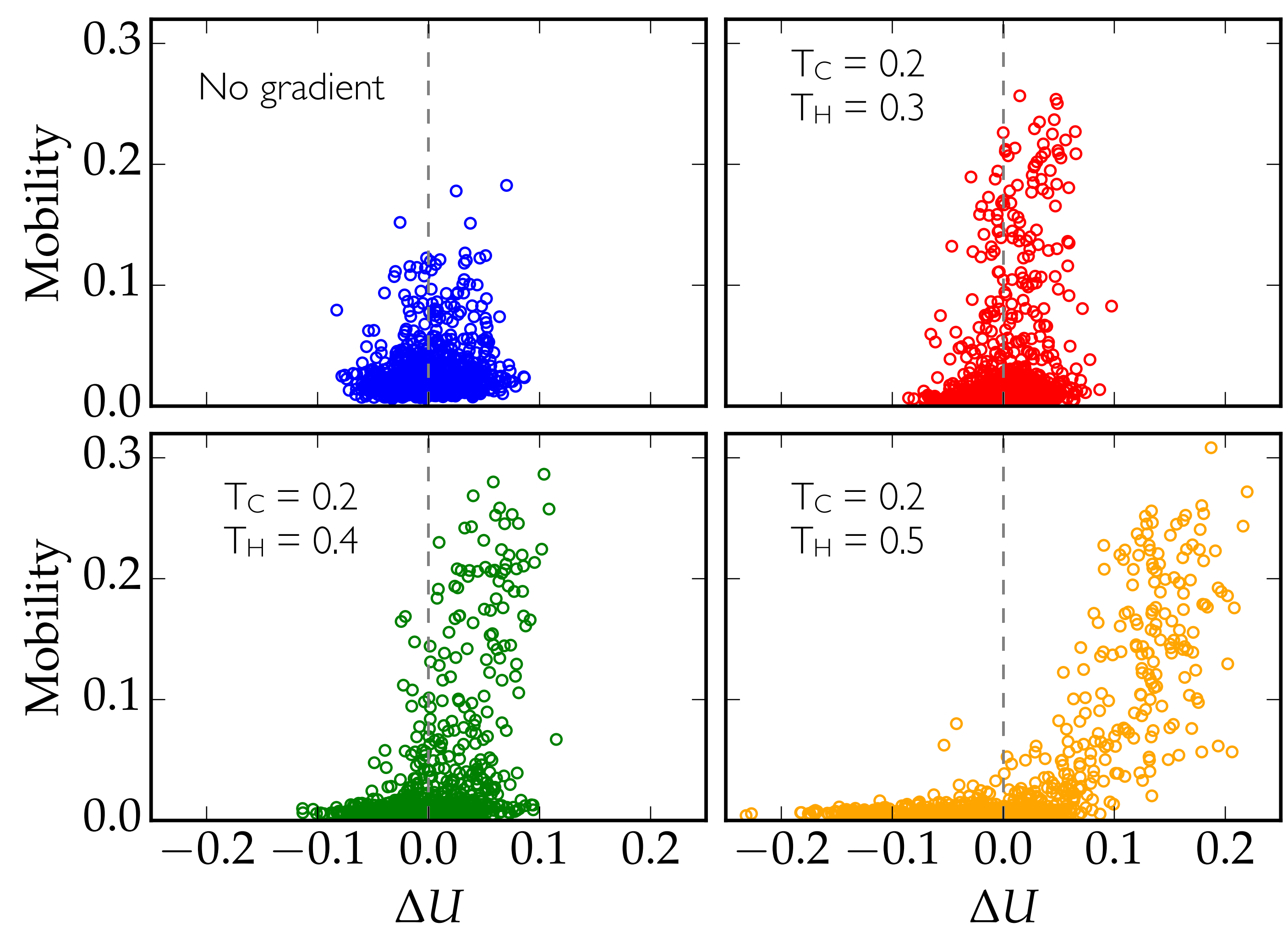
Shear bands in heterogenous samples: position of nucleation



Deforming the heterogeneous samples at fixed shear-rates 10^{-4}

Shear band: region of high mobility
Mobility: squared displacement of particle
Control over the formation of shear-bands?

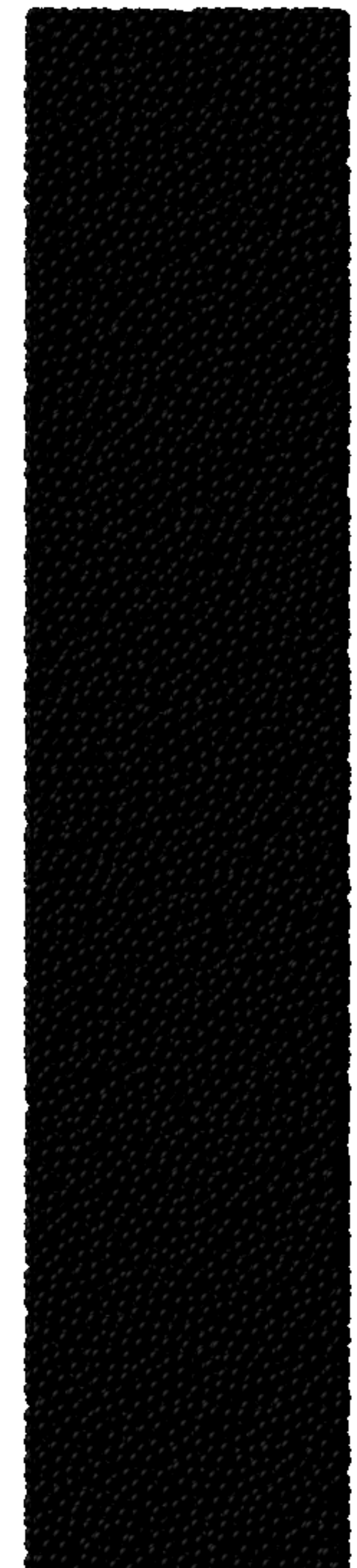
Local mobility (strain = 0.1) vs fluctuation in local potential energy (strain = 0)



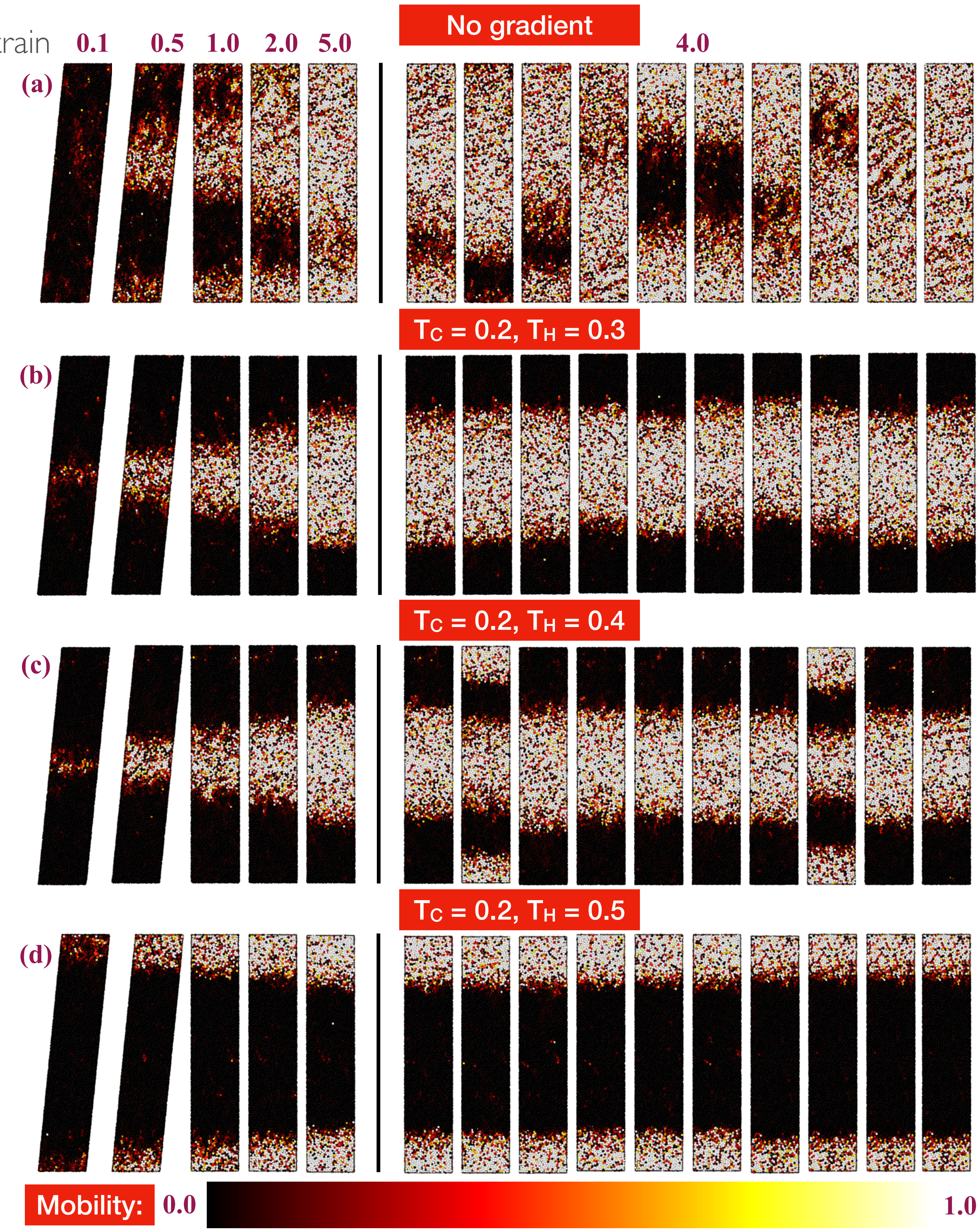
Shear bands in heterogenous samples

Unprocessed sample
T = 0.2

Processed sample
T_c = 0.2 and T_H = 0.5



Shear bands in heterogenous samples: stochastic or deterministic?



10 samples with same initial configuration but different noise of thermostat

Deforming the heterogeneous samples at fixed shear-rate 10^{-4}

Temperature control using DPD thermostat

Checking stochasticity:

— same initial undeformed sample

— change the DPD seed

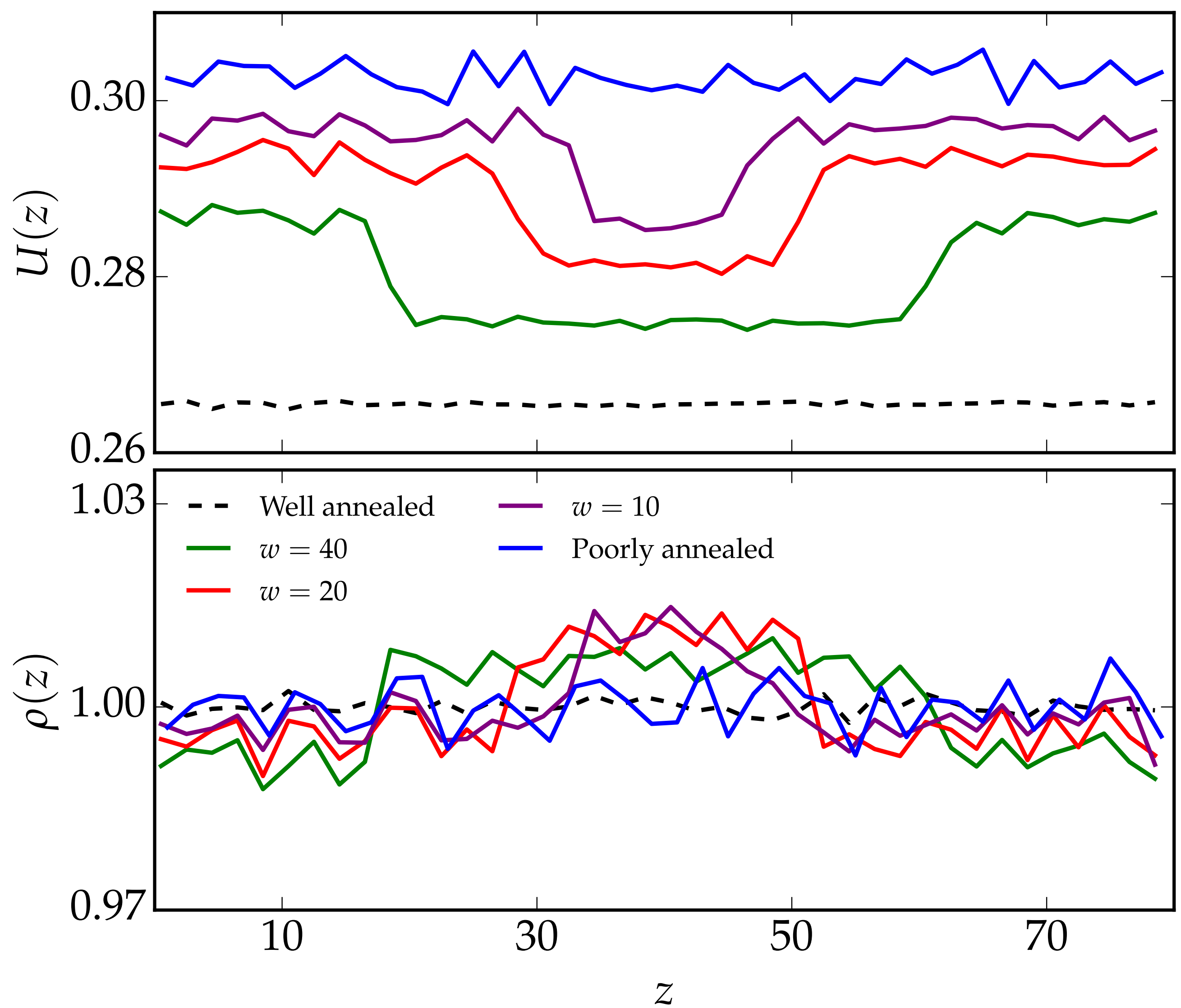
Shear band nucleation is not stochastic if there is sufficient inhomogeneity

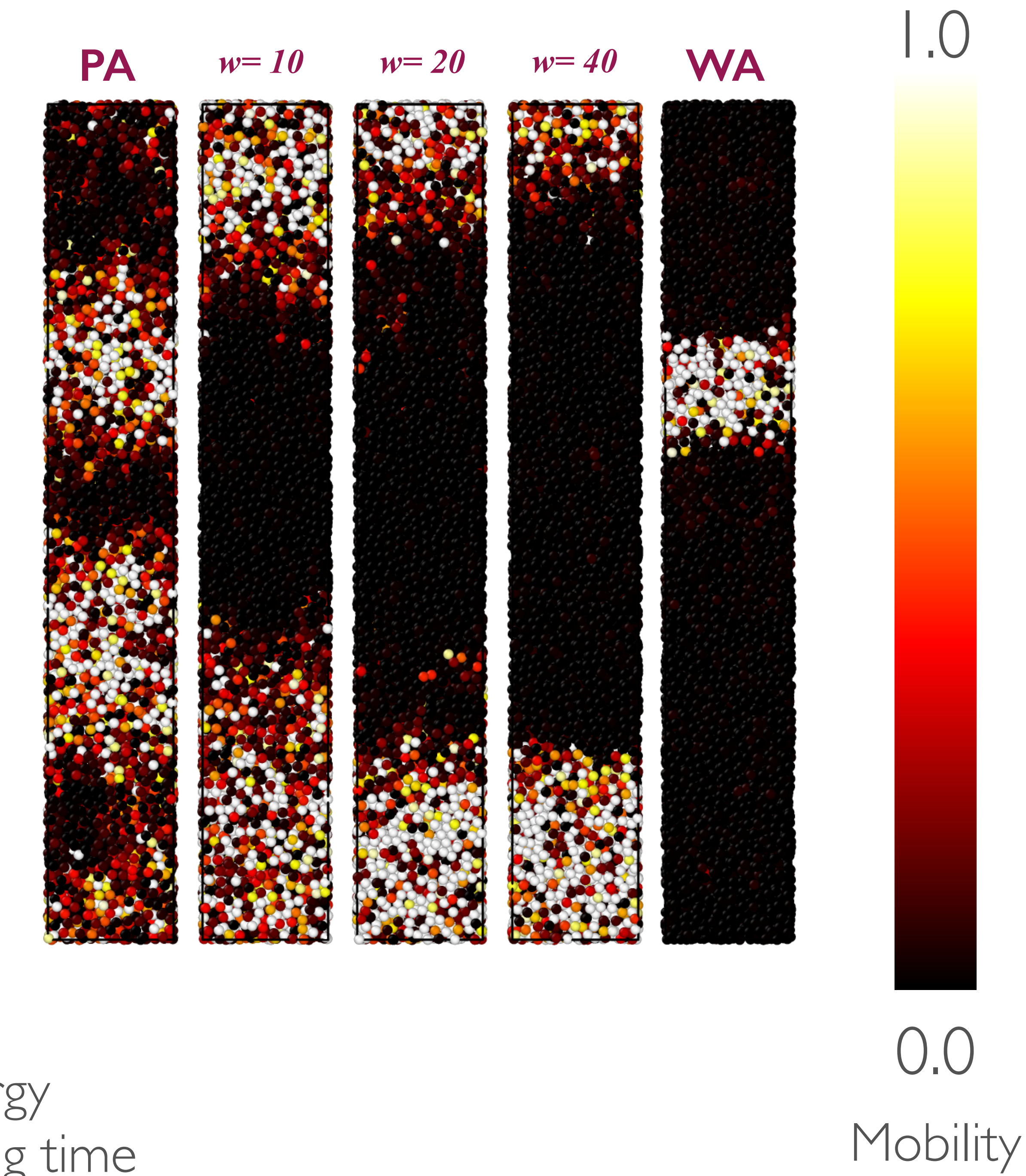
Designing Spatially Inhomogeneous Glasses

Protocol 2: spatially inhomogeneous annealing

— Hybrid swap Monte-Carlo and MD

— swap MC is applied only in central region of width w





Inhomogeneity is dominated by potential energy

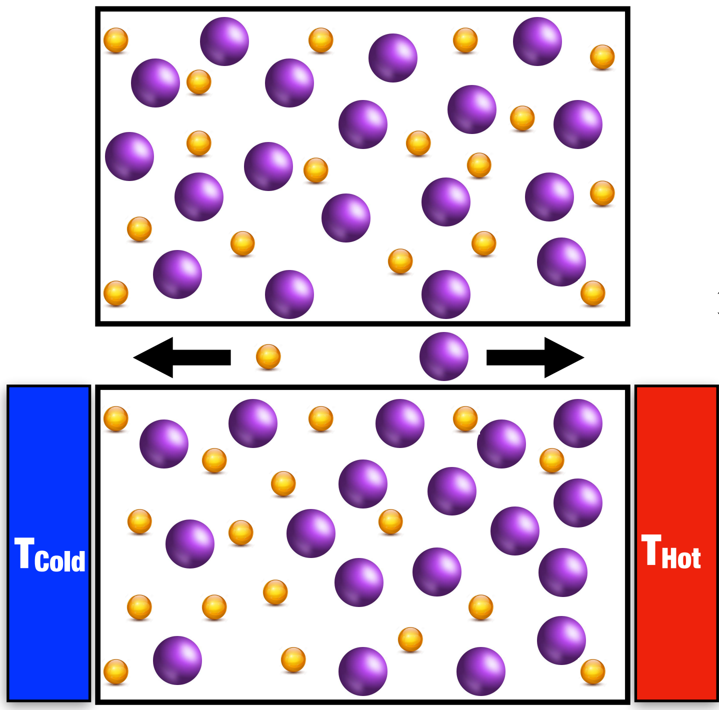
Inhomogeneous structures are stable for a long time

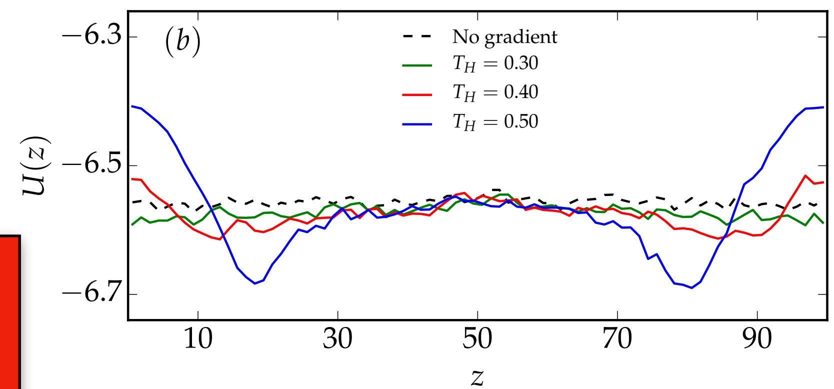
Shear band nucleates in the high energy regions; lifetime is longer

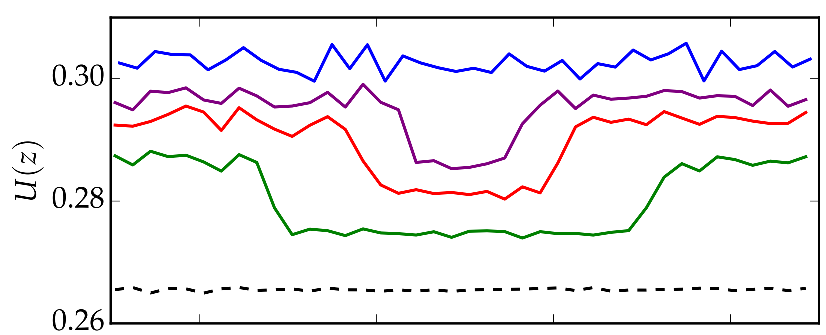
For hybrid swap MC-MD: V. Vaibhav, J. Horbach and P. Chaudhuri; JCP **156**, 244501 (2022)

Summary

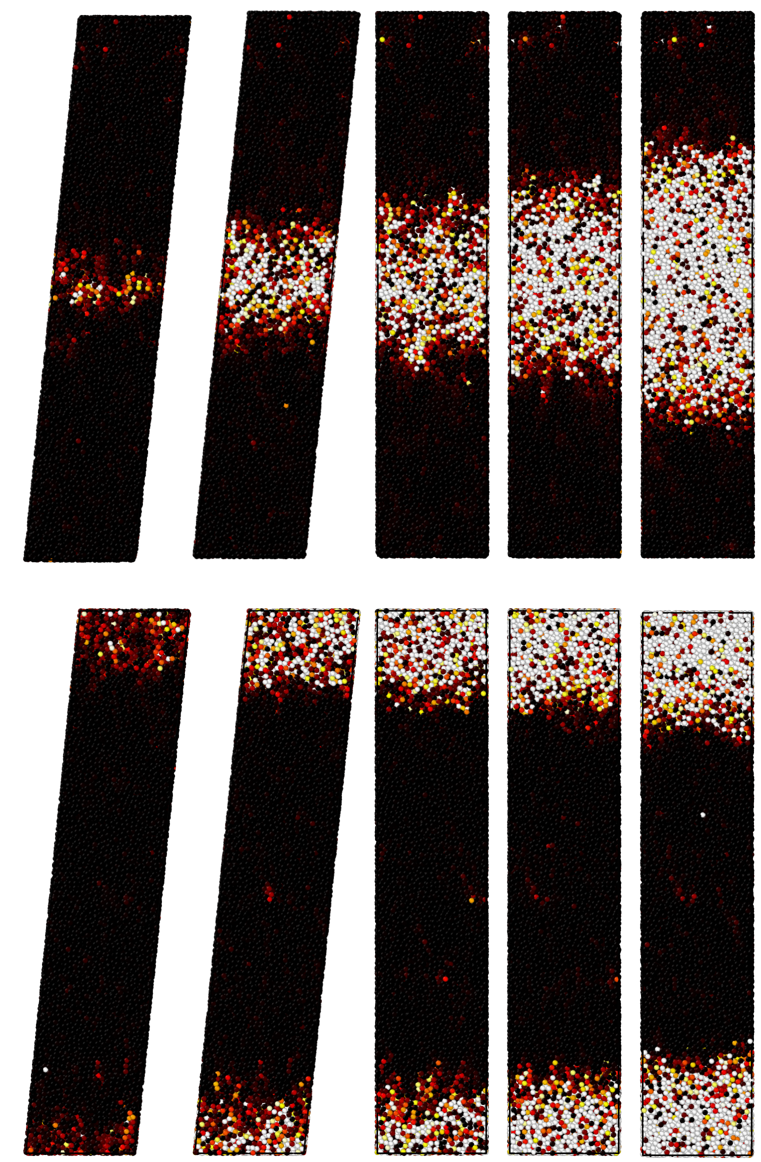
Tuning the spatial inhomogeneity in glasses
— Temperature gradient pulse
— Inhomogeneous annealing







Controlled pathway to failure



Response of glassy liquids to thermal gradients
V. Vaibhav, J. Horbach and P. Chaudhuri; Phys. Rev. E 101, 022605 (2020)

Controlled mechanical failure in glasses via designed spatial inhomogeneity
V. Vaibhav, J. Horbach and P. Chaudhuri; submitted (2023)

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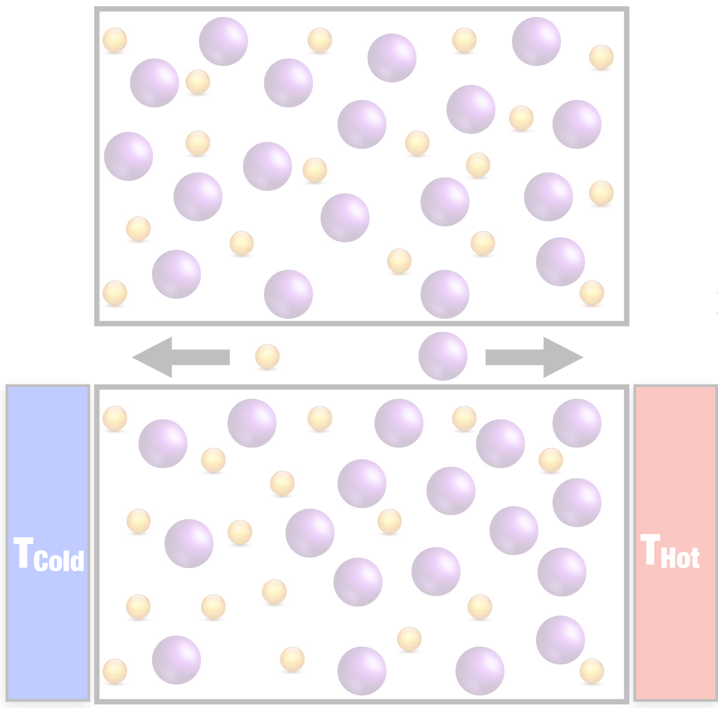

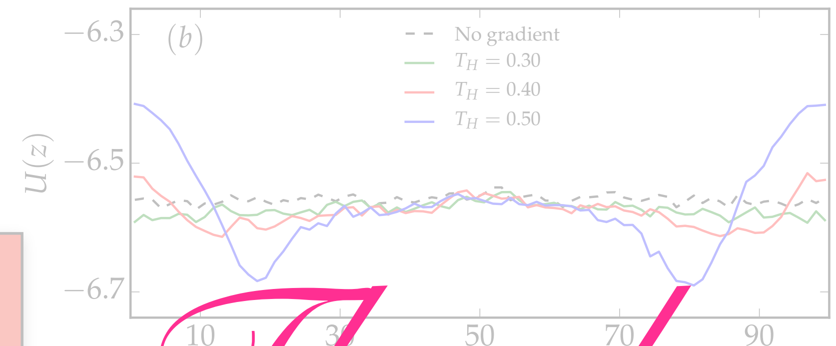

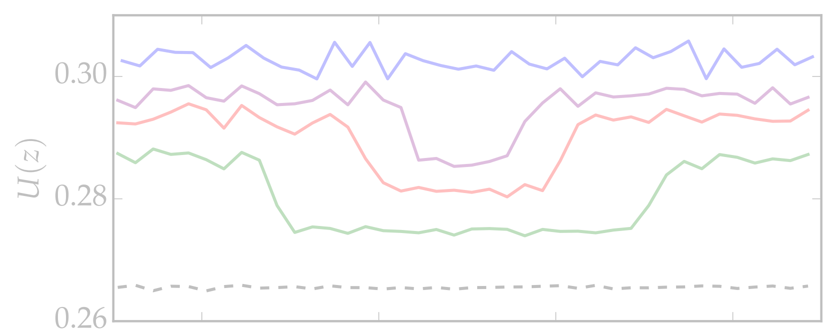

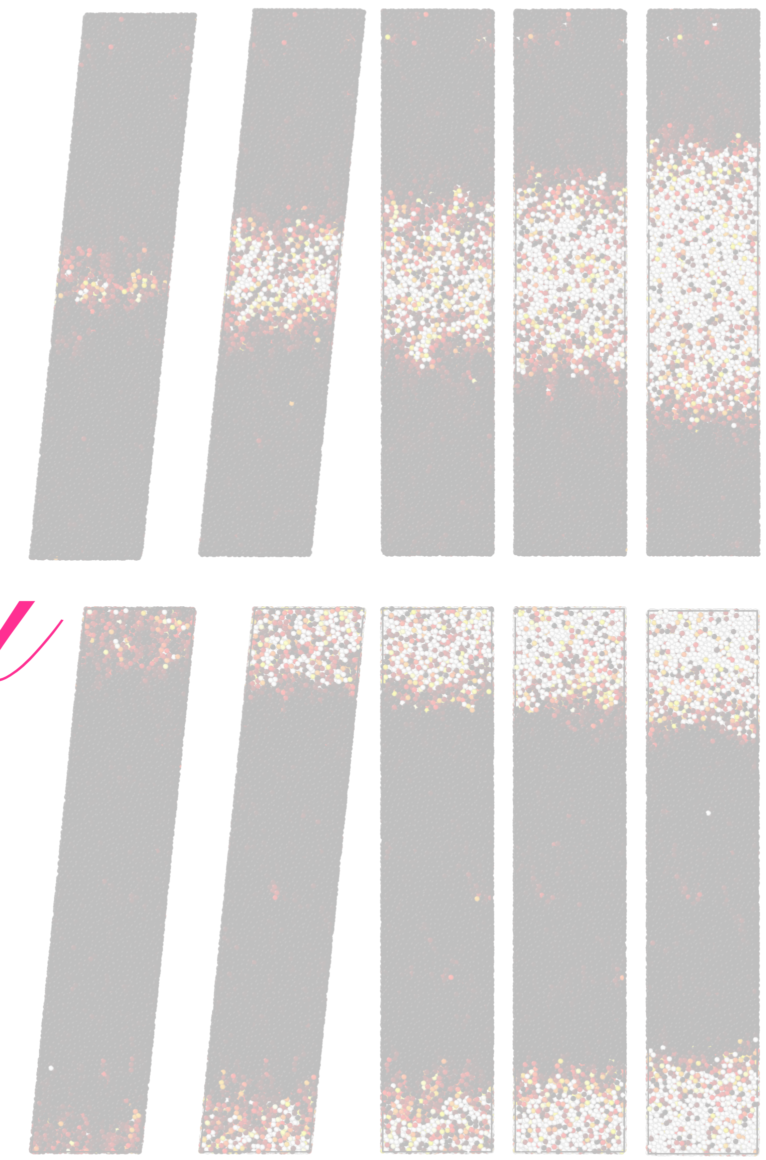

Thank you

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