Heterogeneous dynamics during onset of shear flow in glasses

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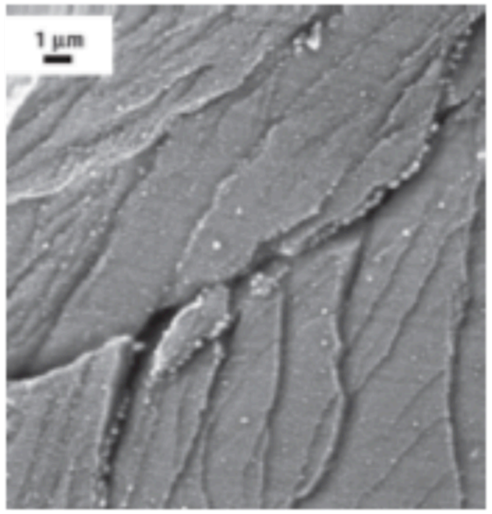
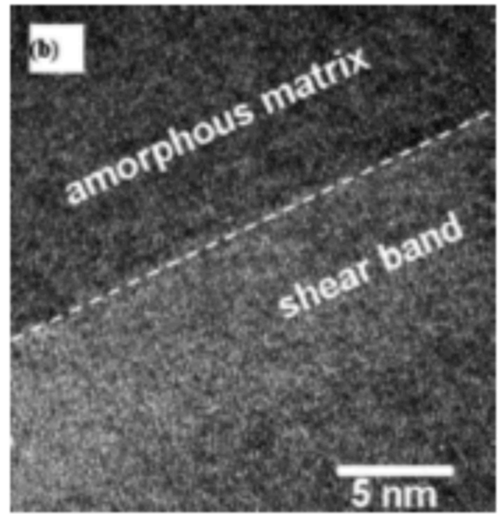
Amorphous solids: inhomogeneous response



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



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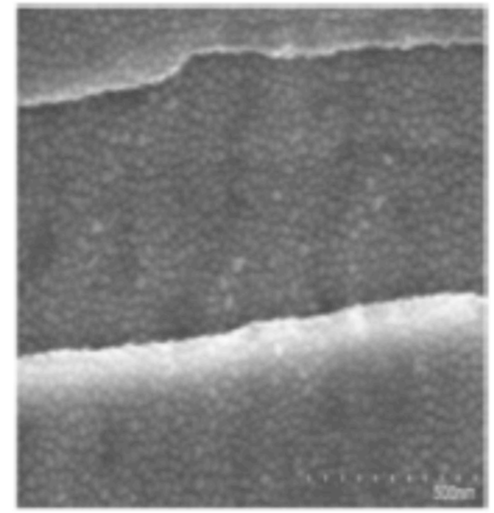
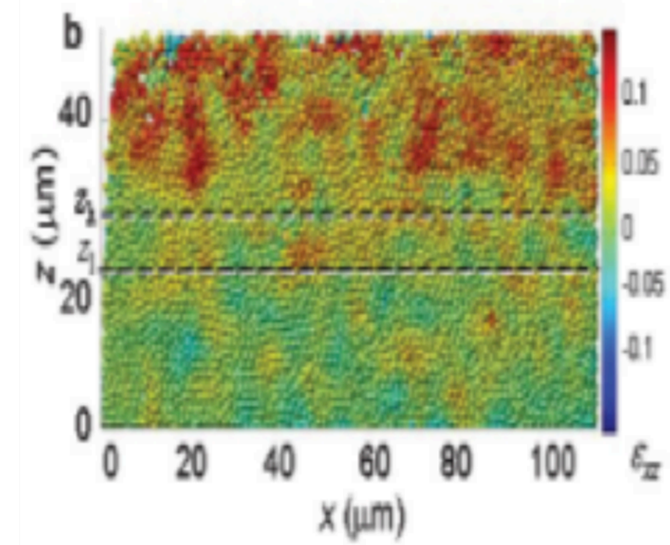
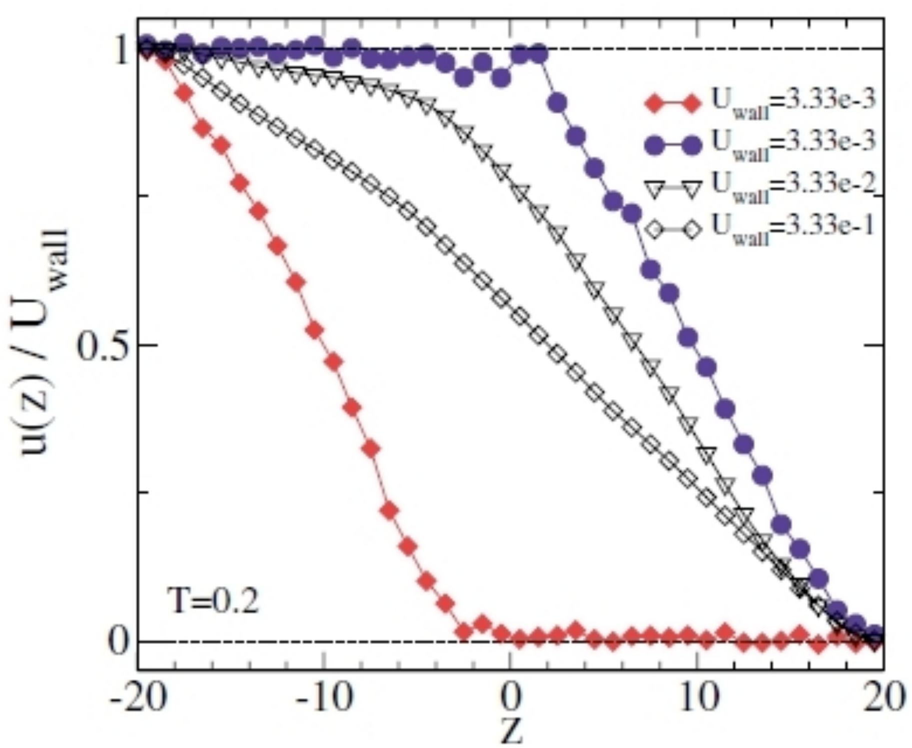


S. V. Ketovet al Sci. Reports 3, 2798 (2013)

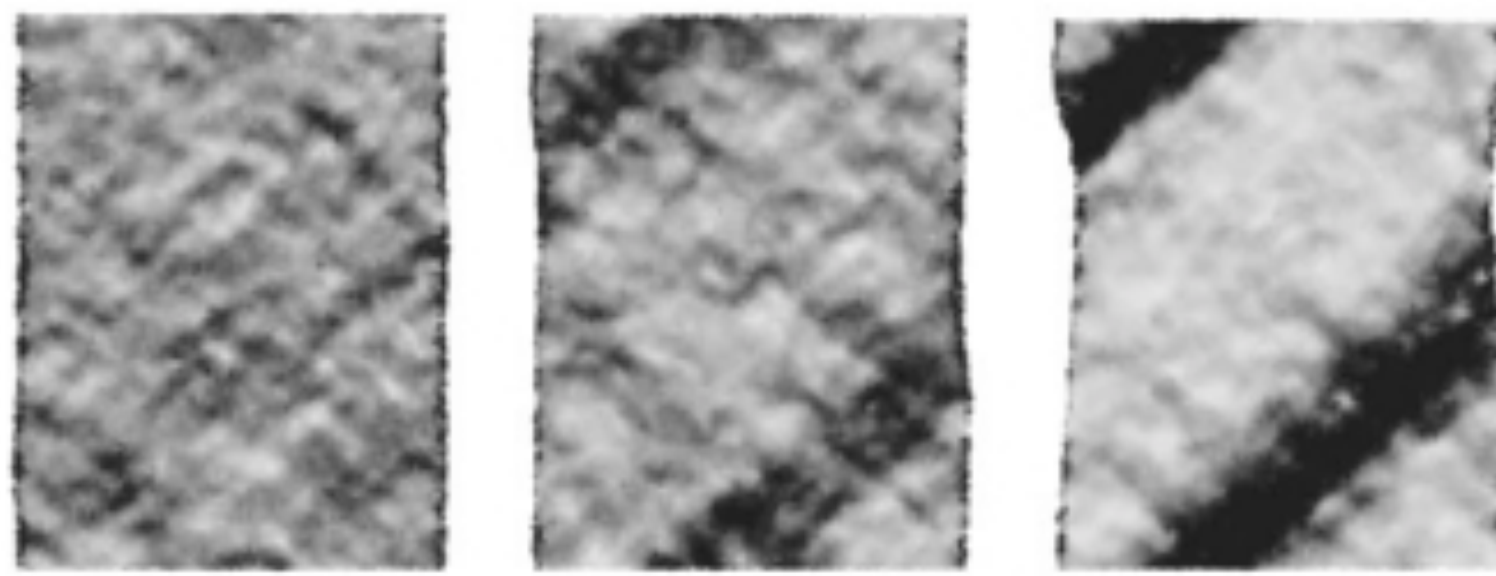


V. Chikkadi et al PRL 107, 198303 (2011)

in numerical simulations



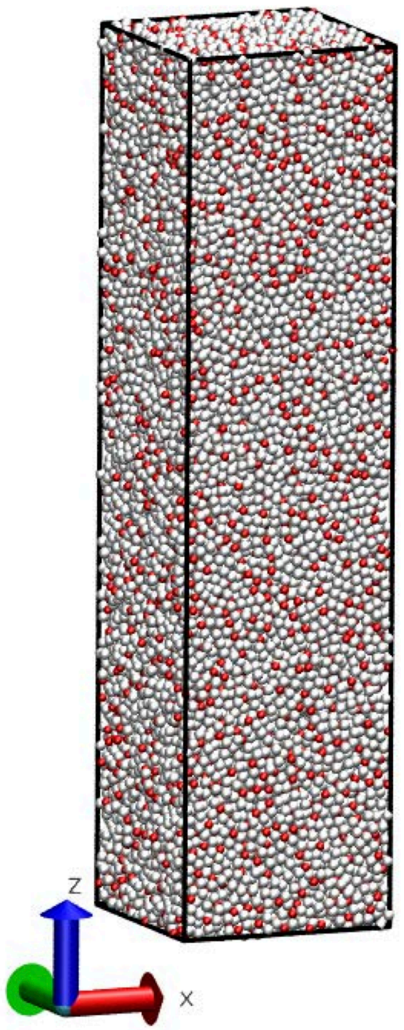
Varnik et al, PRL 2003



Shi et al, PRB 2005

what is the origin? transient/permanent ?

Model and Method



- **Binary mixture of Lennard –Jones particles (A and B) with ratio 80:20**
- **Particles interact via Lennard-Jones potential:**

$$U^{LJ}_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta}\left[(\sigma_{\alpha\beta}/r)^{12} - (\sigma_{\alpha\beta}/r)^{6}\right]$$

where $\alpha, \beta = \mathrm{A, B}$

- **Parameters of the potential are as follows:**

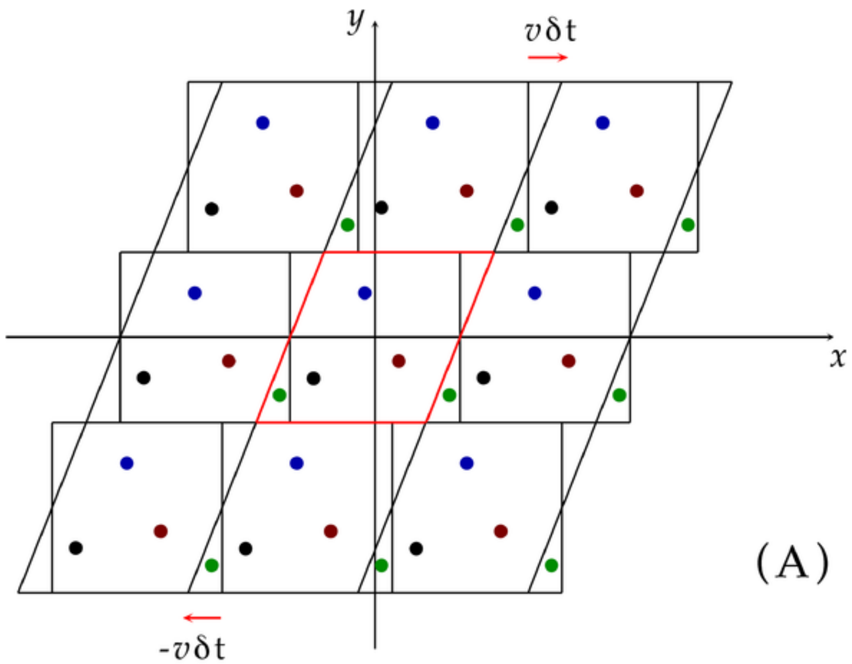
$\epsilon_{AB} = 1.5\epsilon_{AA}$ $\sigma_{AB} = 0.8\sigma_{AA}$ $m_A = m_B$

$\sigma_{BB} = 0.88\sigma_{AA}$ $\epsilon_{BB} = 0.5\epsilon_{AA}$

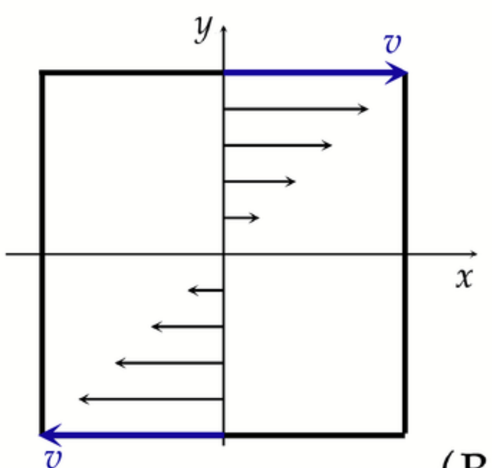
L-J Units	
Length	σ_{AA}
Energy	ε_{AA}
Mass	m_{AA}
Time	$\sigma_{AA}\sqrt{m_A/\varepsilon_{AA}}$

supercooled liquid quenched to glassy temperature (T=0.2), following by aging.

Response to imposed shear-rate monitored.

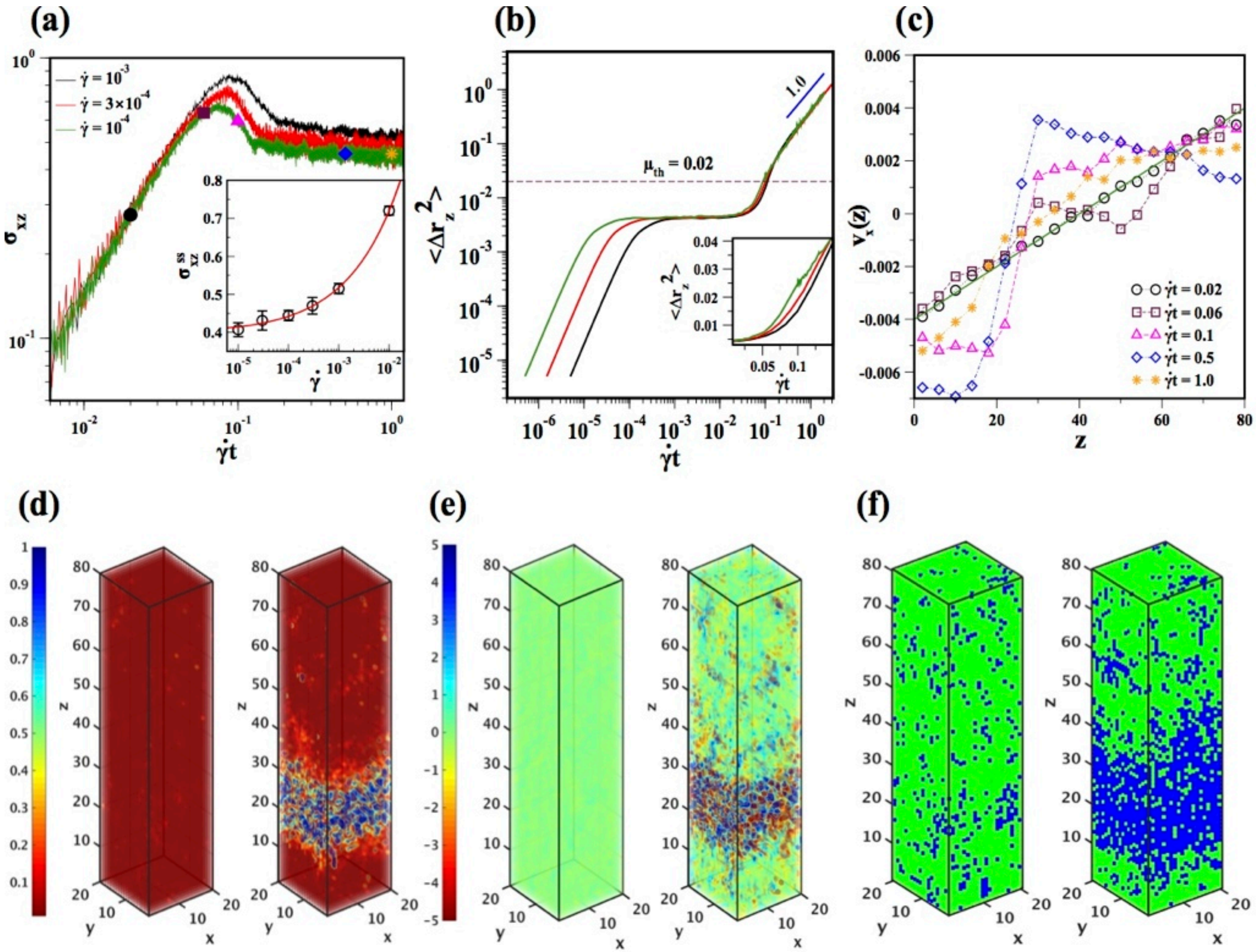


(A)



(B)

Response to imposed shear-rate at finite T

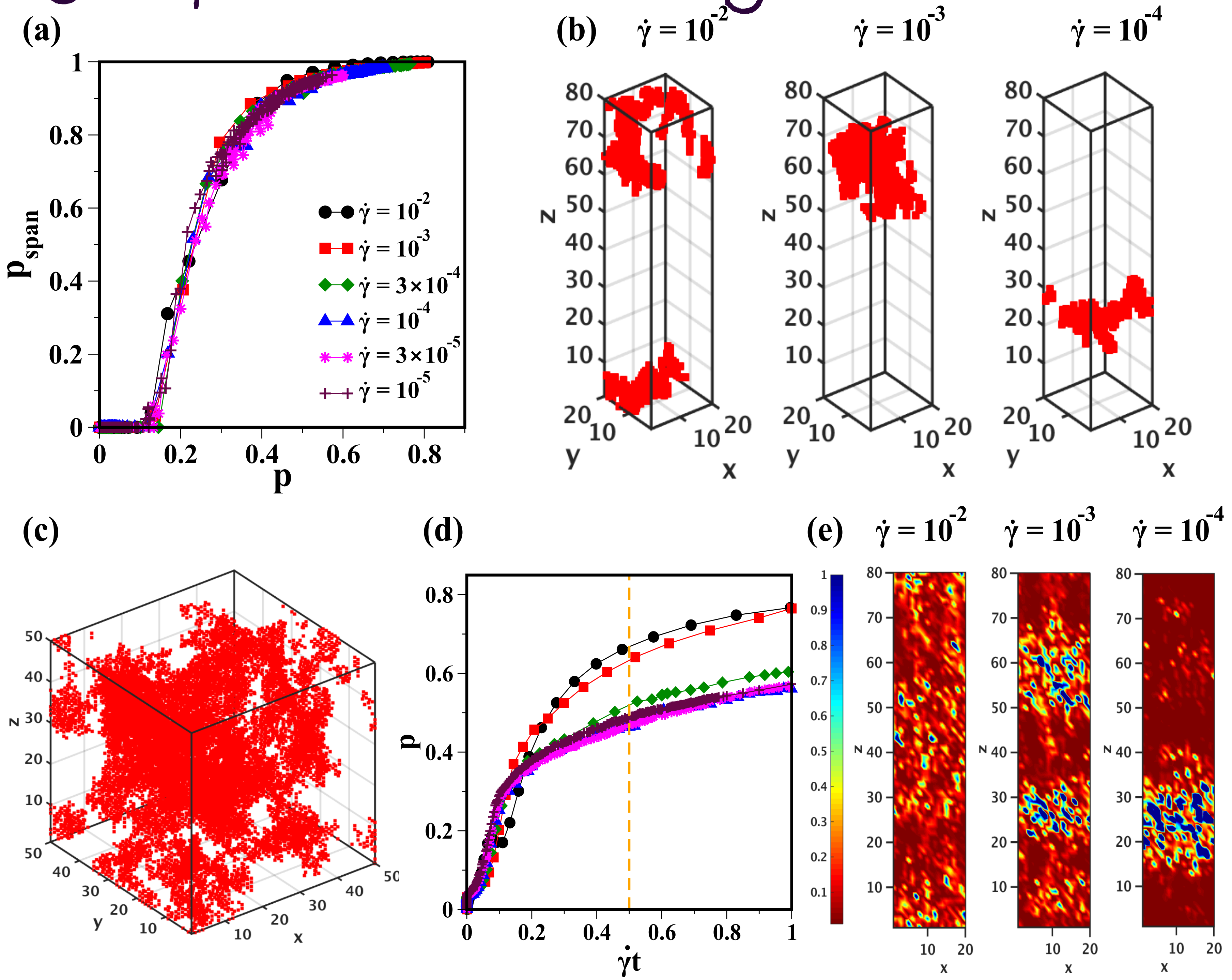


characteristic macro response (stress-overshoot); mapped to single particle displacements

fluctuating velocity profiles; alternative probe: displacement with respect to quiescent state; maps similar to strain field

region deemed active if displacement above a threshold; cluster analysis of active regions.

Yielding: a percolation analysis - I

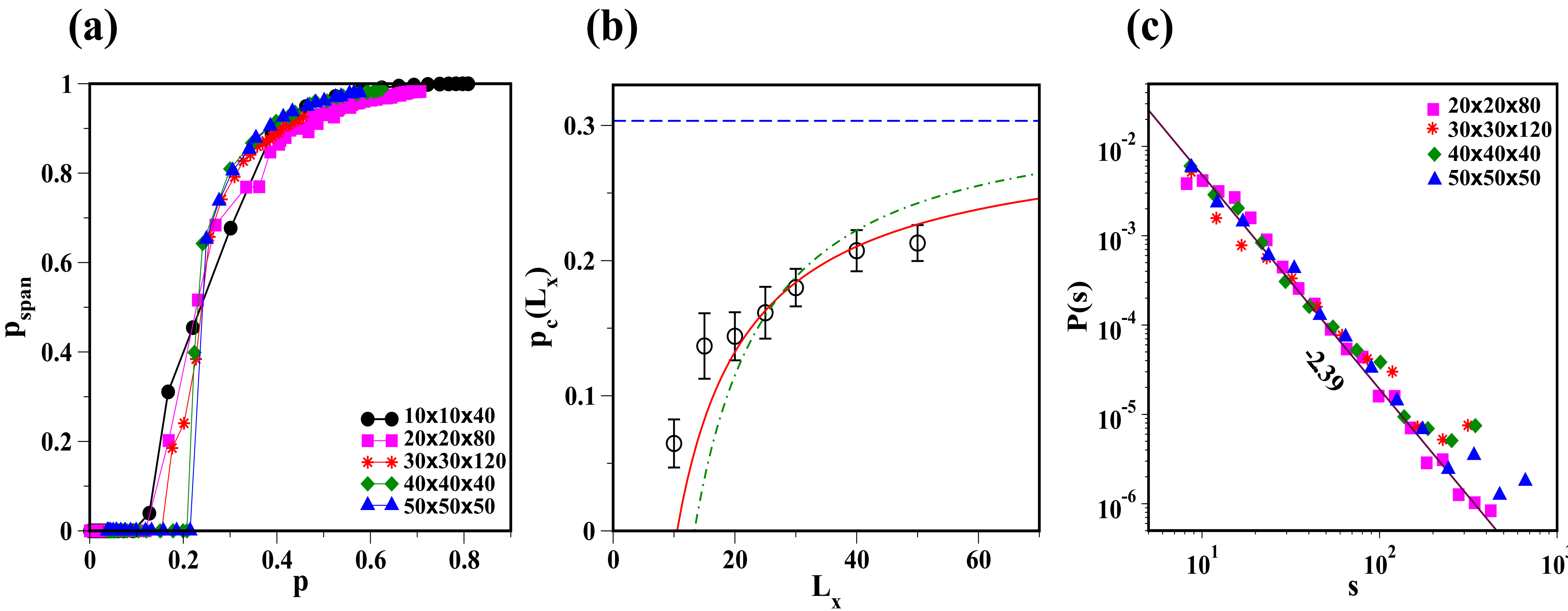


active sites percolate for all imposed shear-rates, at strains corresponding to stress-overshoot.

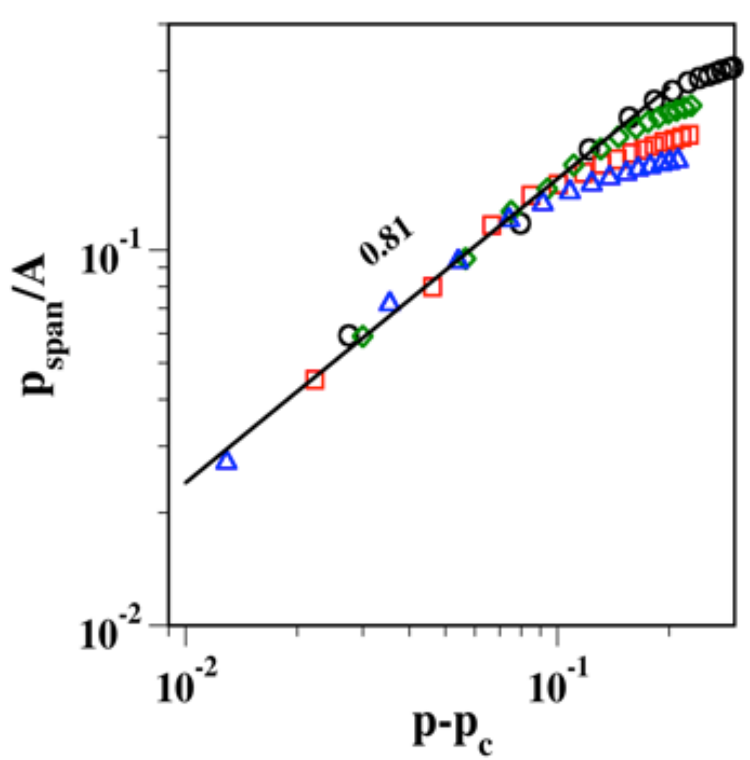
percolating cluster a 3d fractal object - finite size effects can localize clustering.

beyond percolation, growth of active sites independent on imposed shear-rate; observation of further heterogeneities at small shear-rates.

Yielding: a percolation analysis - II



Exponents		
	DP	SP
$p_c(\infty)$	0.3033	0.3116
$\vartheta_{\|\|}$	1.106	0.87
τ	2.39	2.18

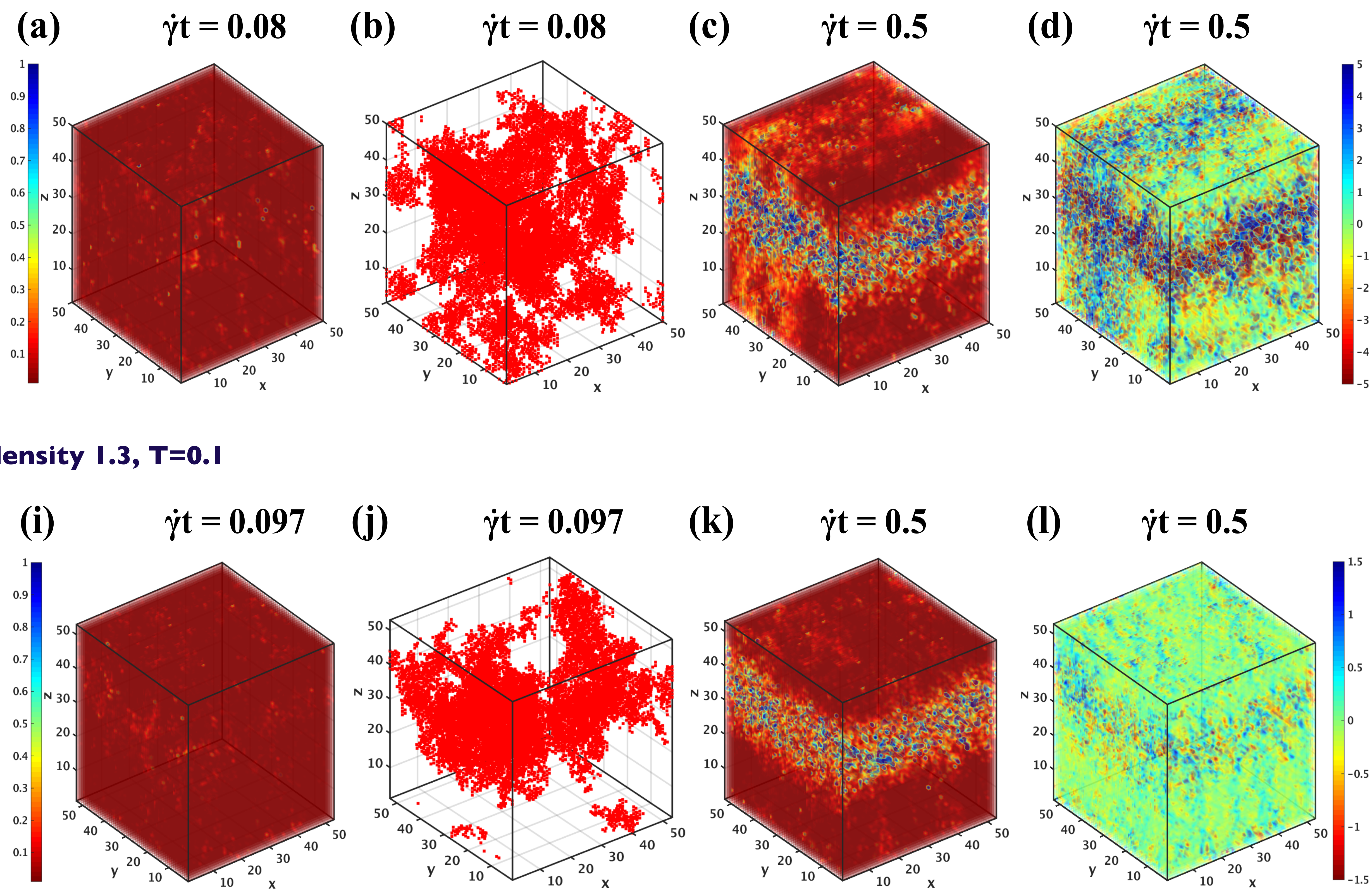


finite-size scaling analysis of percolation threshold as well as distribution cluster sizes indicate possible directed percolation scenario.

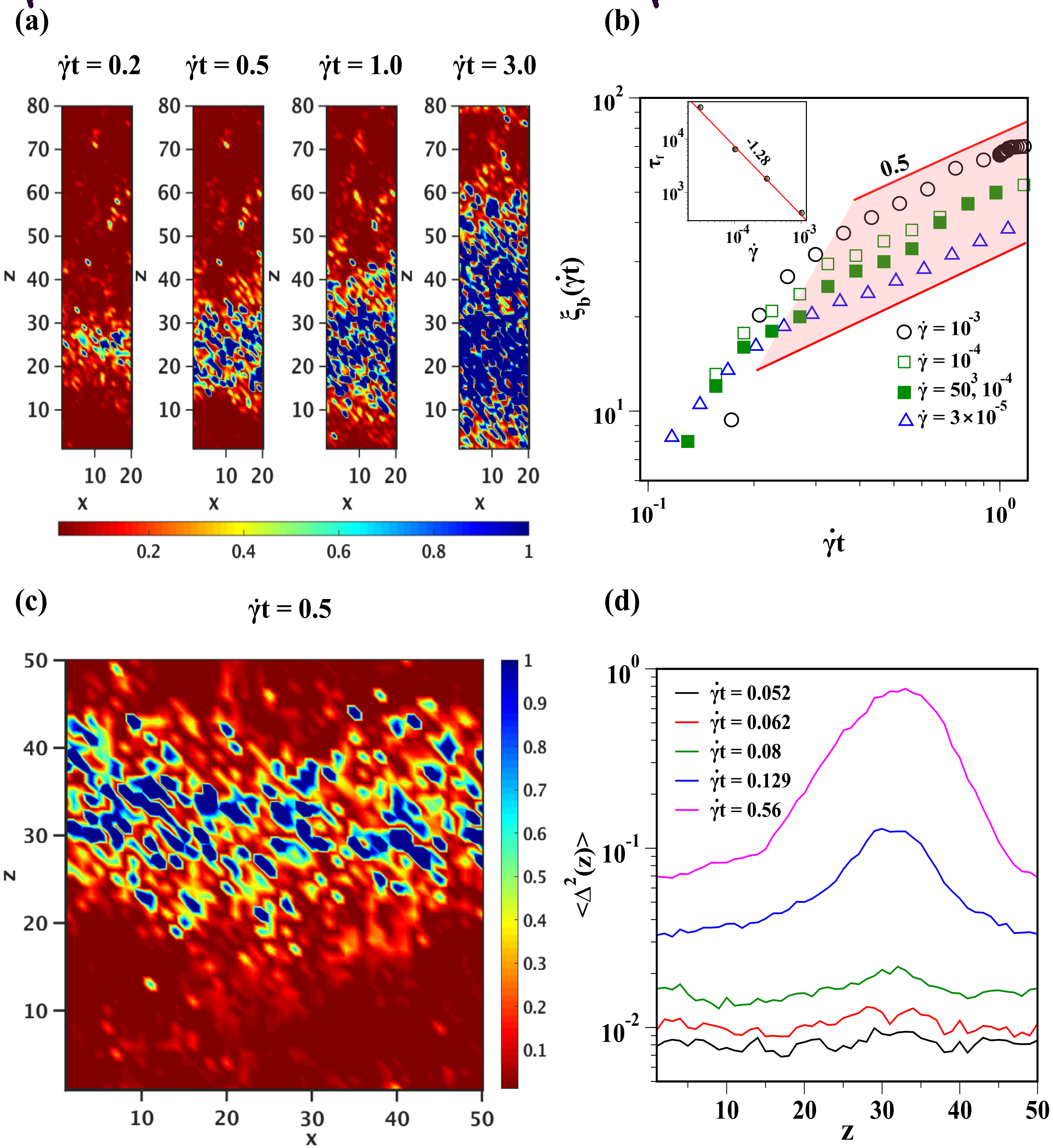
Post-percolation: emergence of shearbands

density 1.2, T=0.2

density 1.3, T=0.1

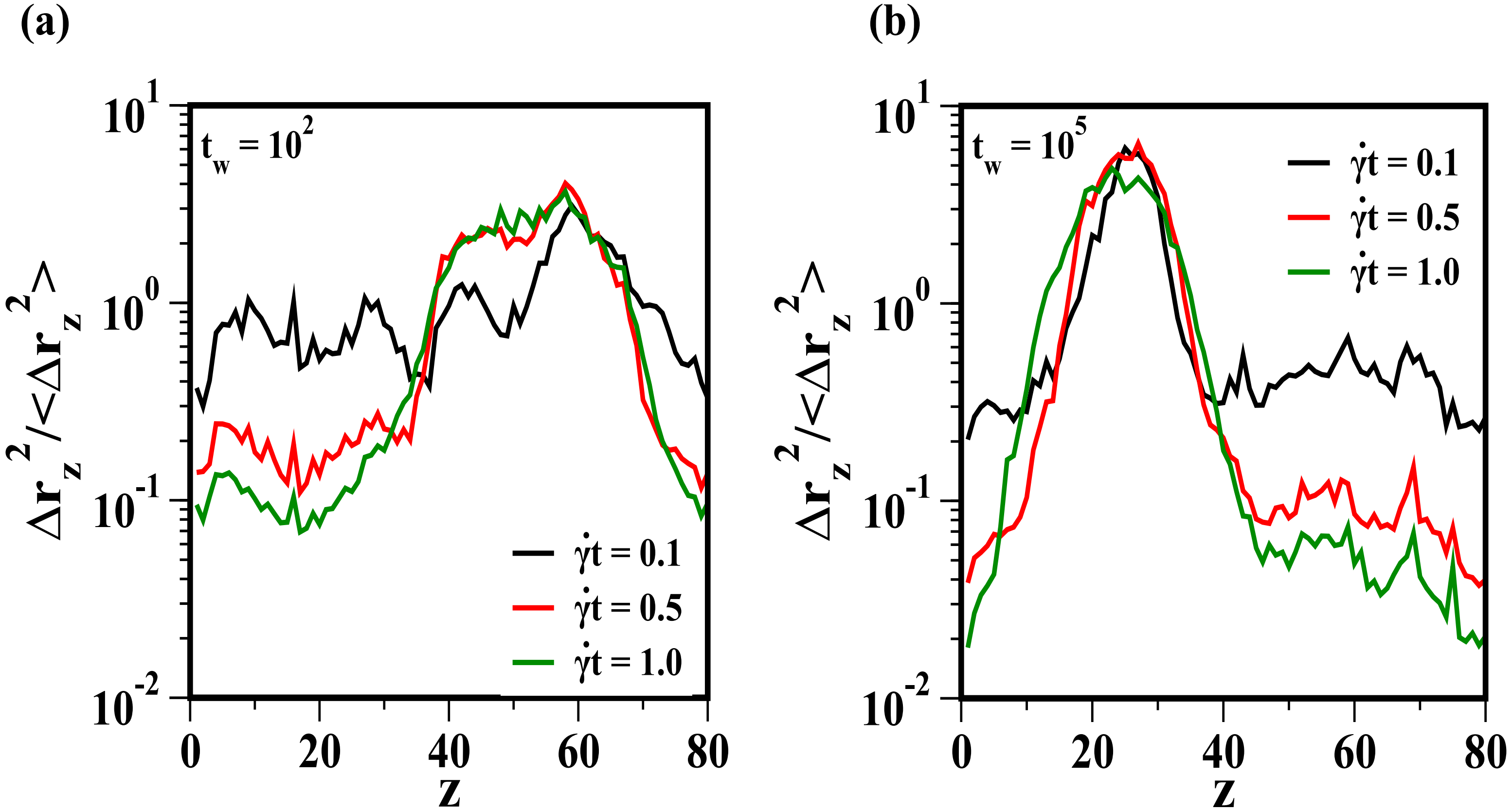


Mobility of shear-band interface



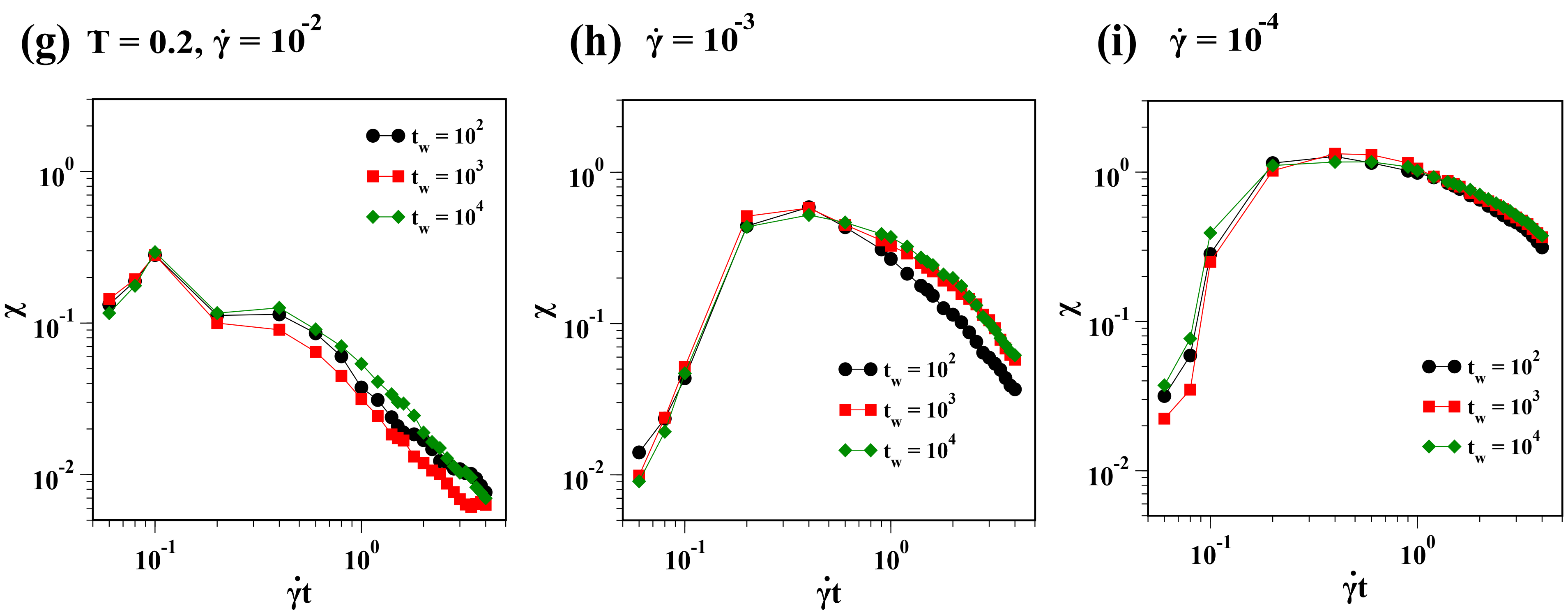
identify shearband interface; roughness depends on temperature
diffusive growth of shearband width; depends on imposed shear-rate;
fluidisation timescales diverge with decreasing shear-rate

Transient heterogeneities: quantifying fluctuations

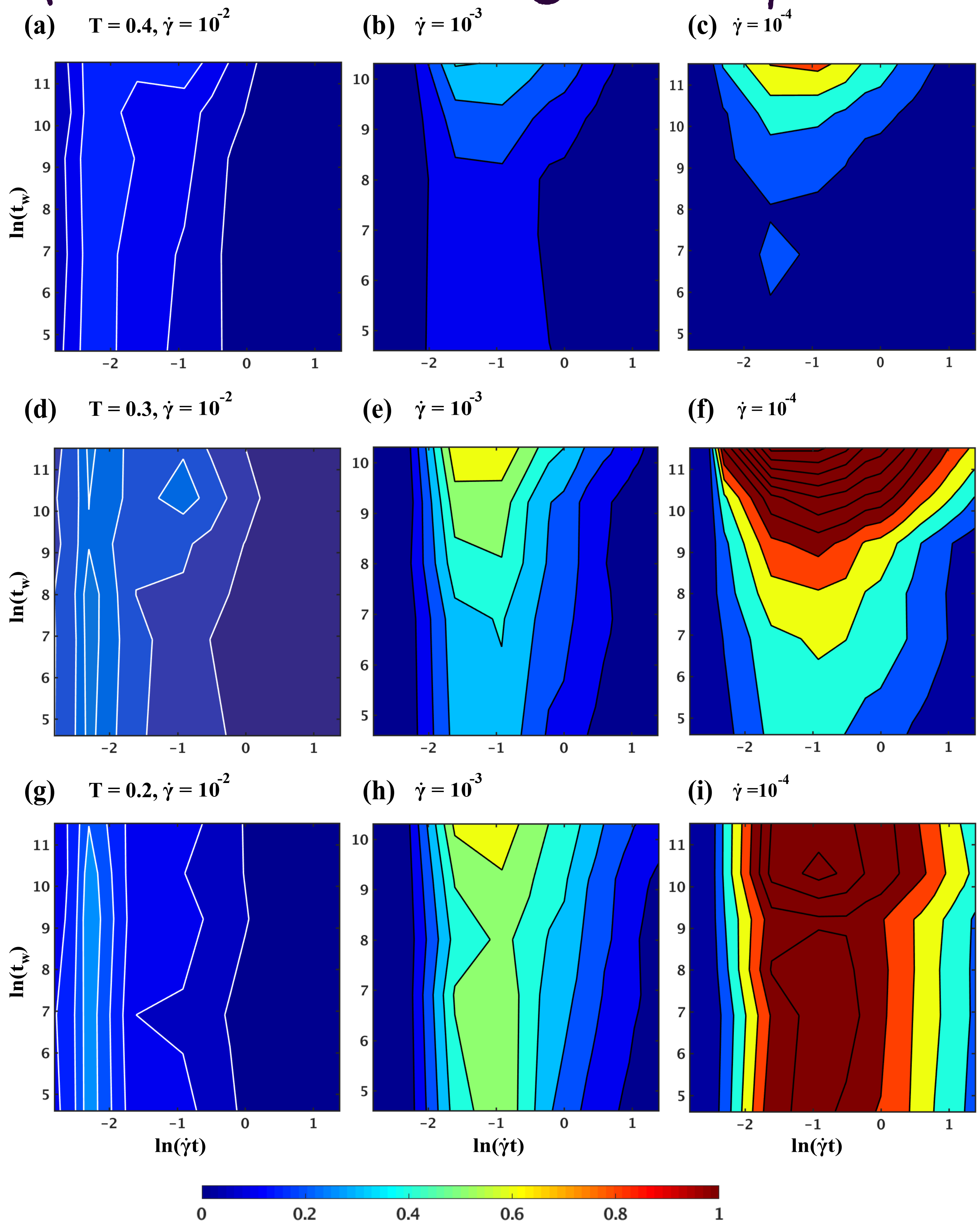


measuring spatial variance in local MSD across layers parallel to direction of external drive

fluctuations non-monotonic with strain duration; maximal at emergence of shear-band; peak-height increases with age, decreasing shear-rate.



Transient fluctuations: age, temperature..



occurrence of shearbands: prominent with low temperature, low shear-rate, longer ages.

Conclusion

onset of flow in glass studied for different imposed shear rates.
occurrence of transient flow heterogeneities
yielding associated with a percolation of active sites: directed percolation ?
shearbands emerge, for small shear-rates, after percolation
transient heterogeneities related to aging, external drive, temperature.
similar to dynamical heterogeneities in quiescent supercooled liquids

References

* GP Shrivastav, P Chaudhuri, J Horbach, Journal of Rheology 60 (5), 835 [2016]
* GP Shrivastav, P Chaudhuri, J Horbach, Physical Review E 94 (4), 042605 [2016]

future work: extend to other shear protocols (with S. Sastry); micro-meso modeling (with K. Martens)