MICROSTRUCTURAL MEMORY IN AMORPHOUS SOLIDS: STZ DEFECTS AND CONFIGURATIONAL TEMPERATURE FIELDS

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  - Michael Shields (Hopkins)
  - Damien Vandembroucq (ESPCI)

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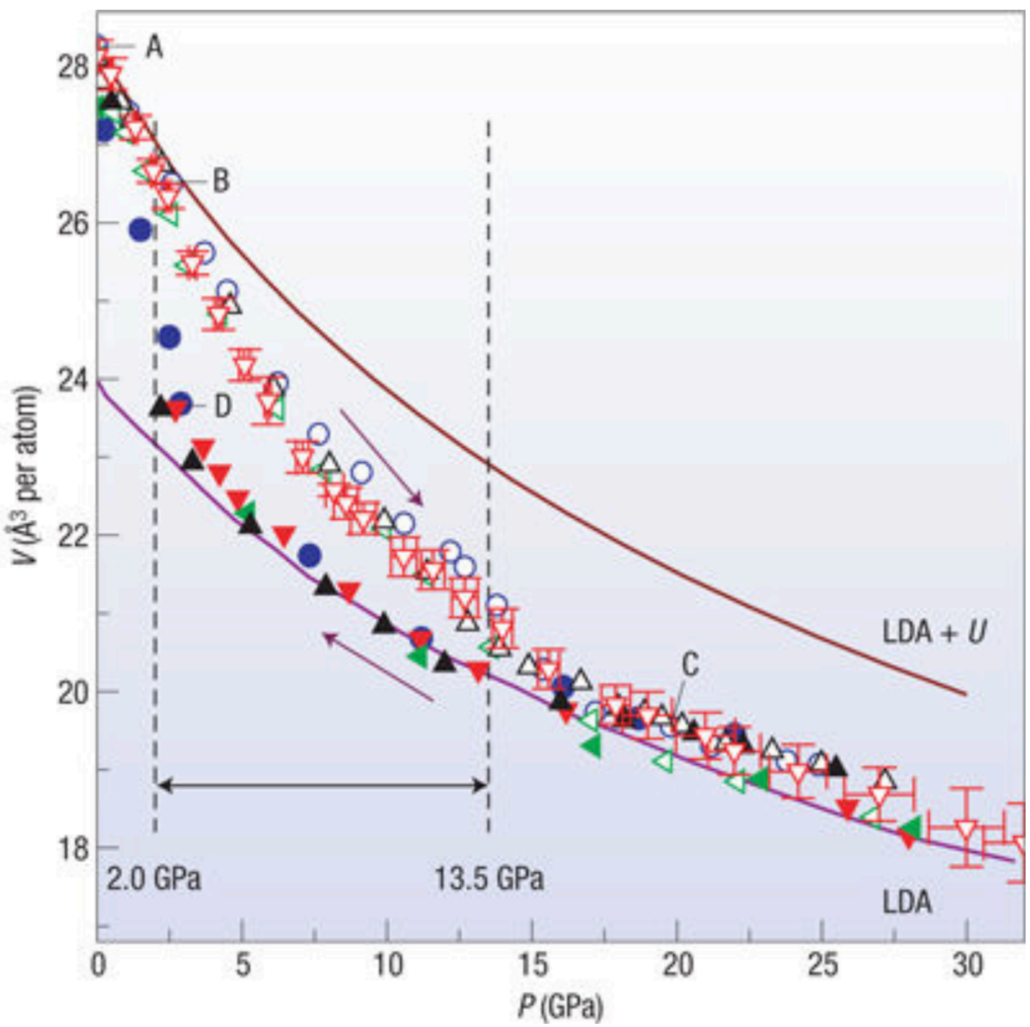
THE MEMORIES OF AMORPHOUS SOLIDS

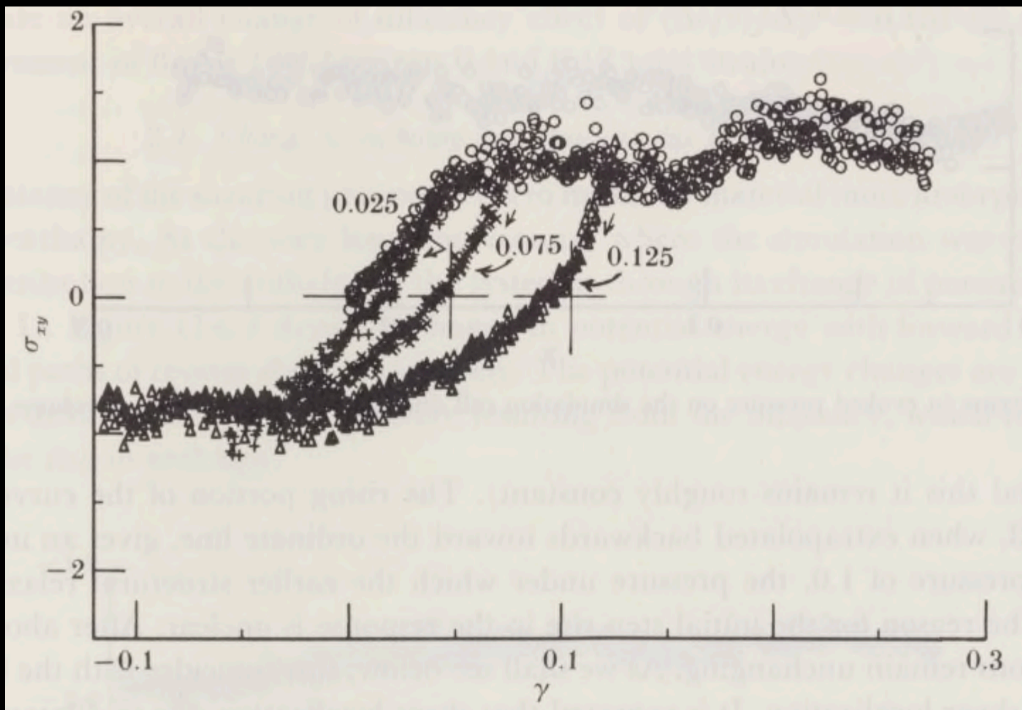
Figure 2: Specific volume versus pressure for amorphous $Ce_{55}Al_{45}$.

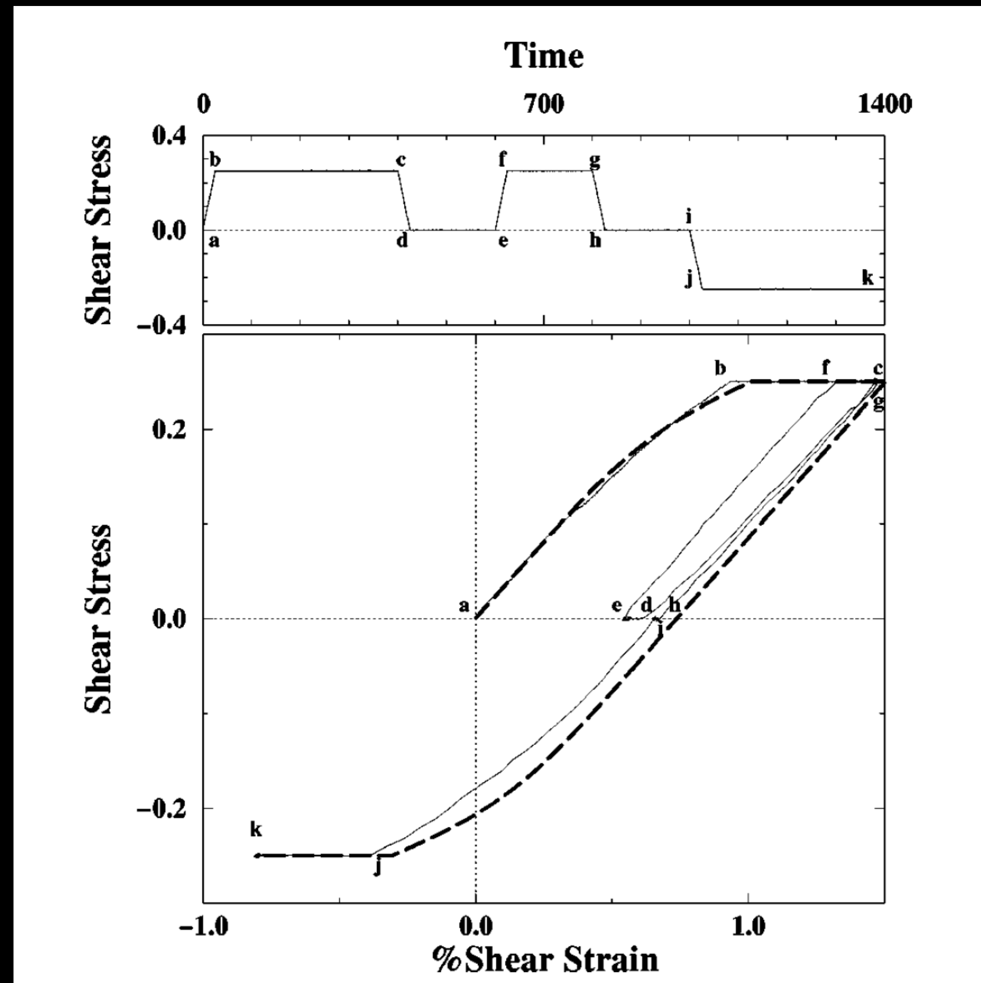


Polyamorphism in a metallic glass

Sheng, Liu, Cheng, Wen, Lee, Luo, Shastri, Ma, Nature Materials, 6, 192–197 (2007)

THE MEMORIES OF AMORPHOUS SOLIDS





Bauschinger Effects in glass simulations

Deng, Argon, Yip, Phil Trans R Soc London A, 329, 613 (1989)

Falk, Langer, Physical Review E, 57, 7192 (1998)

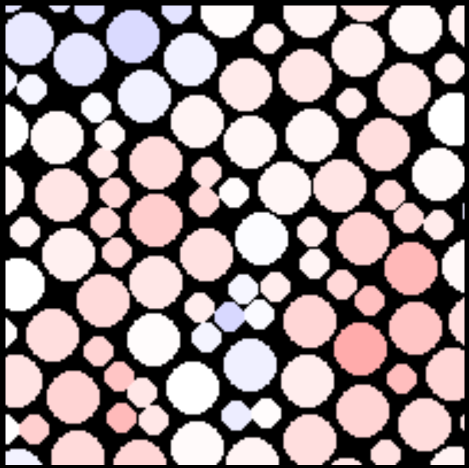
SHEAR TRANSFORMATION ZONES

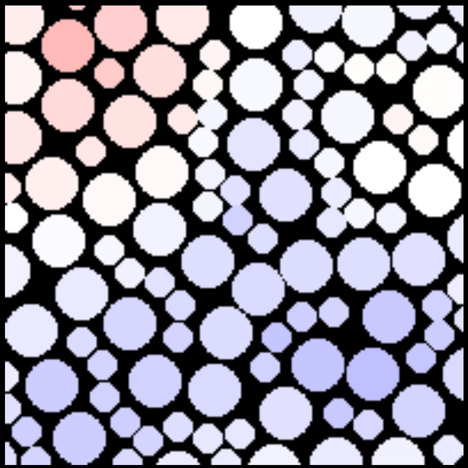
A MICRO-MECHANISM FOR PLASTICITY

FALK, LANGER, PRE 57, 7192 (1998)

- LOCAL - ORIENTATIONAL -

- PERSISTENT - SELF-GENERATING -





SPAEPEN (1977)

FLOW DEFECTS

LOCAL - PERSISTENT -
FREE VOLUME MEDIATED

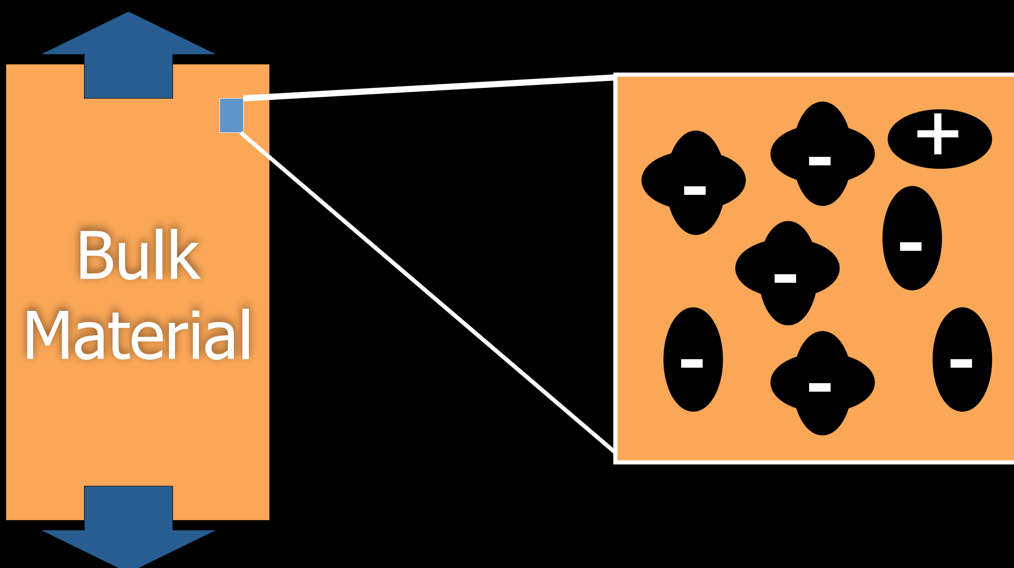
ARGON (1979)

SHEAR TRANSFORMATION

LOCAL - ORIENTATIONAL -
FREE VOLUME MEDIATED

STZ CONSTITUTIVE THEORY

FALK, LANGER, PRE 57, 7192 (1998); ARCMP 2, 353 (2011)



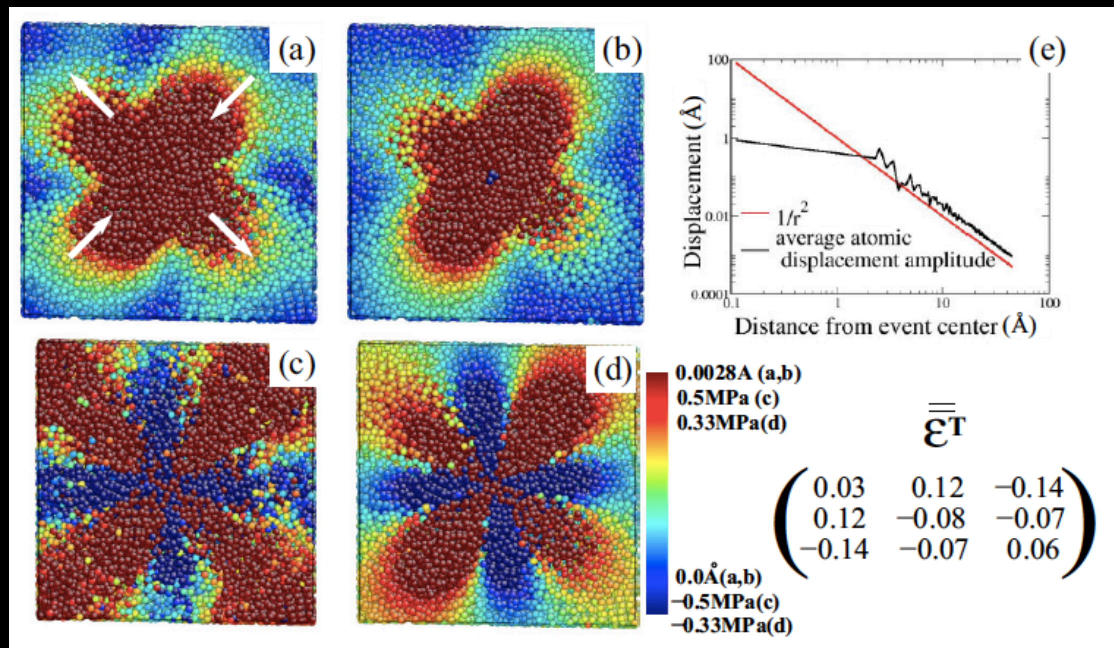
- External strain induces elastic stress.
- Elastic stress causes STZs to transform, resulting in plastic strain.
- STZ transformation events induce STZ creation and annihilation.

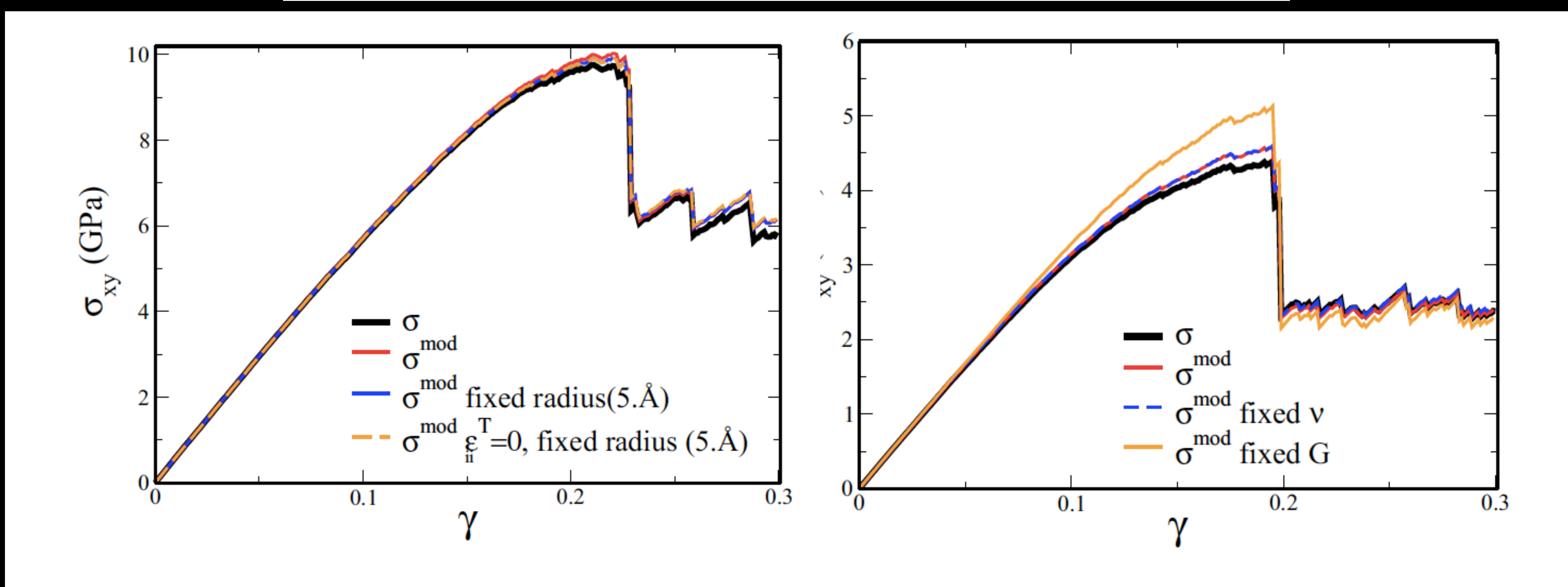
CAN THE STZ HYPOTHESIS BE CONFIRMED BY ATOMISTIC SIMULATION?

- **Are the defects truly Eshelby-like?**
  YES: Albaret, Tanguy, Boioli and Rodney, PRE 93 053002 (2016)
- **Are they *a priori* detectable in aspects of the structure?**
  - **Phonon Spectra**: Manning, Liu, PRL 107, 108302 (2011); Schoenholz, Liu, Riggleman, Rottler PRX 4, 031014 (2014)
  - **Topological SRO**: Ding, Patinet, Falk, Cheng, Ma, PNAS 111, 14052 (2014); and numerous other works
  - **Short Range Spatial Correlations**: Cubuk, Schoenholz, Rieser, Malone, Rottler, Durian, Kaxiras, Liu, PRL 114, 108001 (2015)
  - **Local Yield Response**: Patinet, Vandembroucq and Falk, PRL 117, 045501 (2016)

ARE THE DEFECTS TRULY ESHELBY-LIKE?

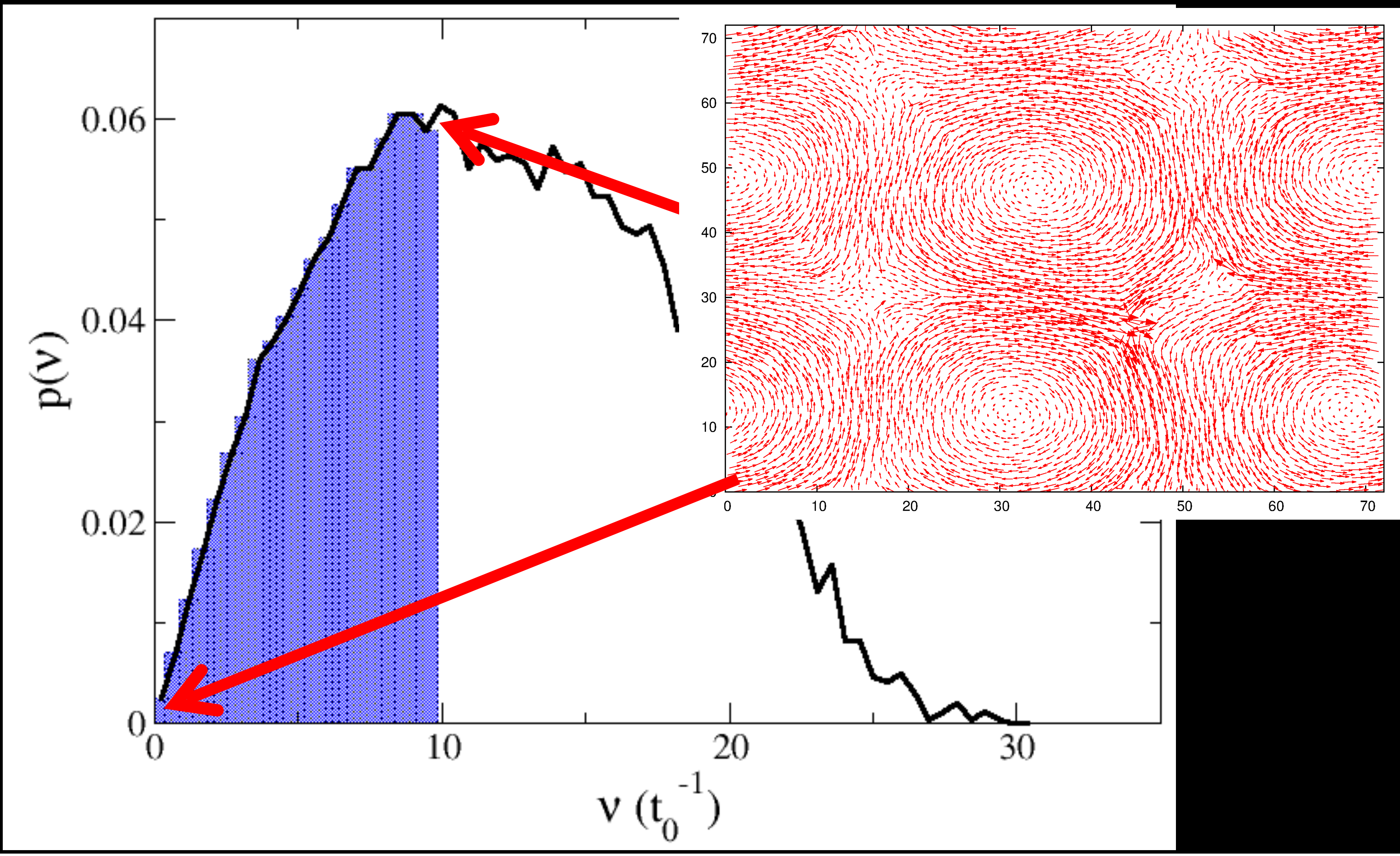
ALBARET, TANGUY, BOIOLI AND RODNEY, PRE 93 053002 (2016)





NORMAL MODE ANALYSIS

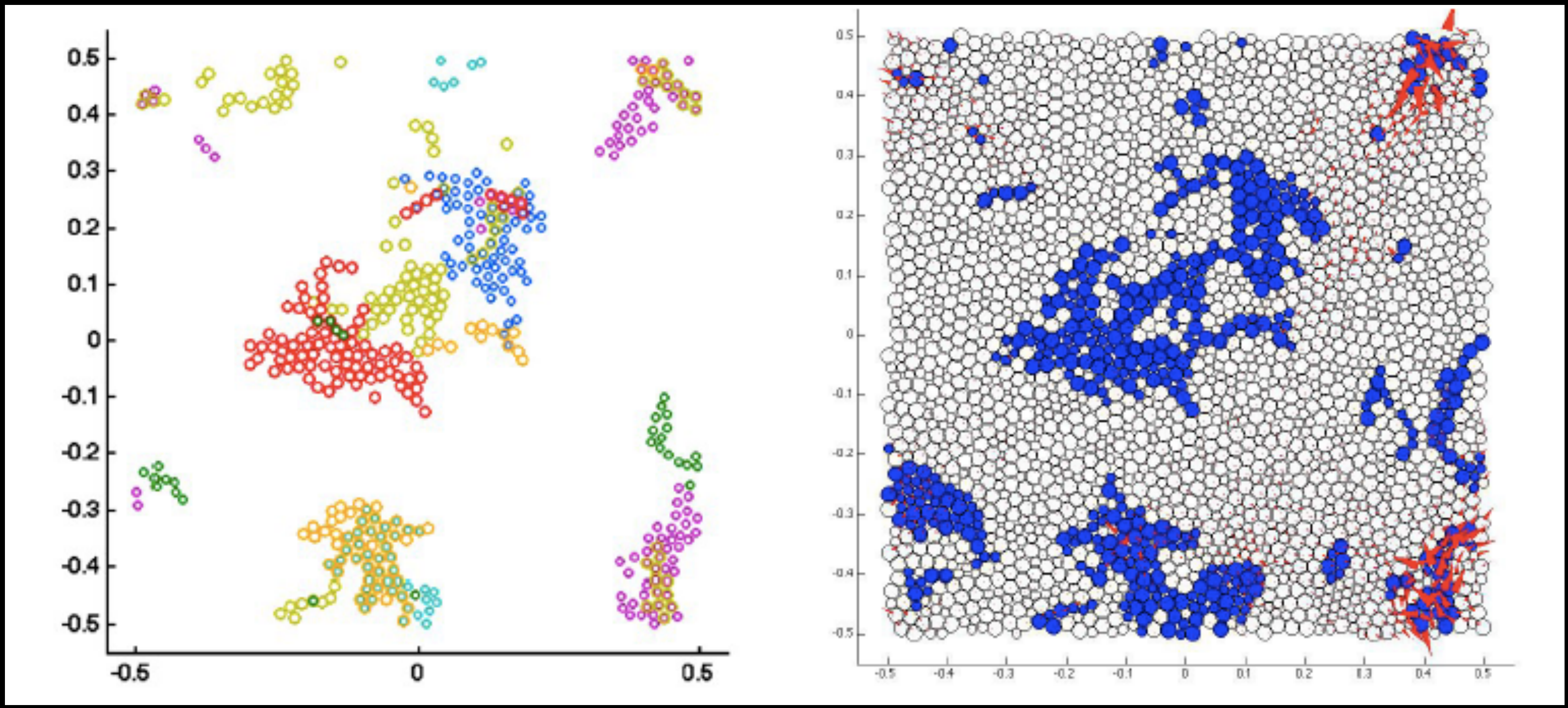
MANNING, LIU, PRL 107, 108302 (2011)



EVIDENCE FOR SHEAR TRANSFORMATION ZONES

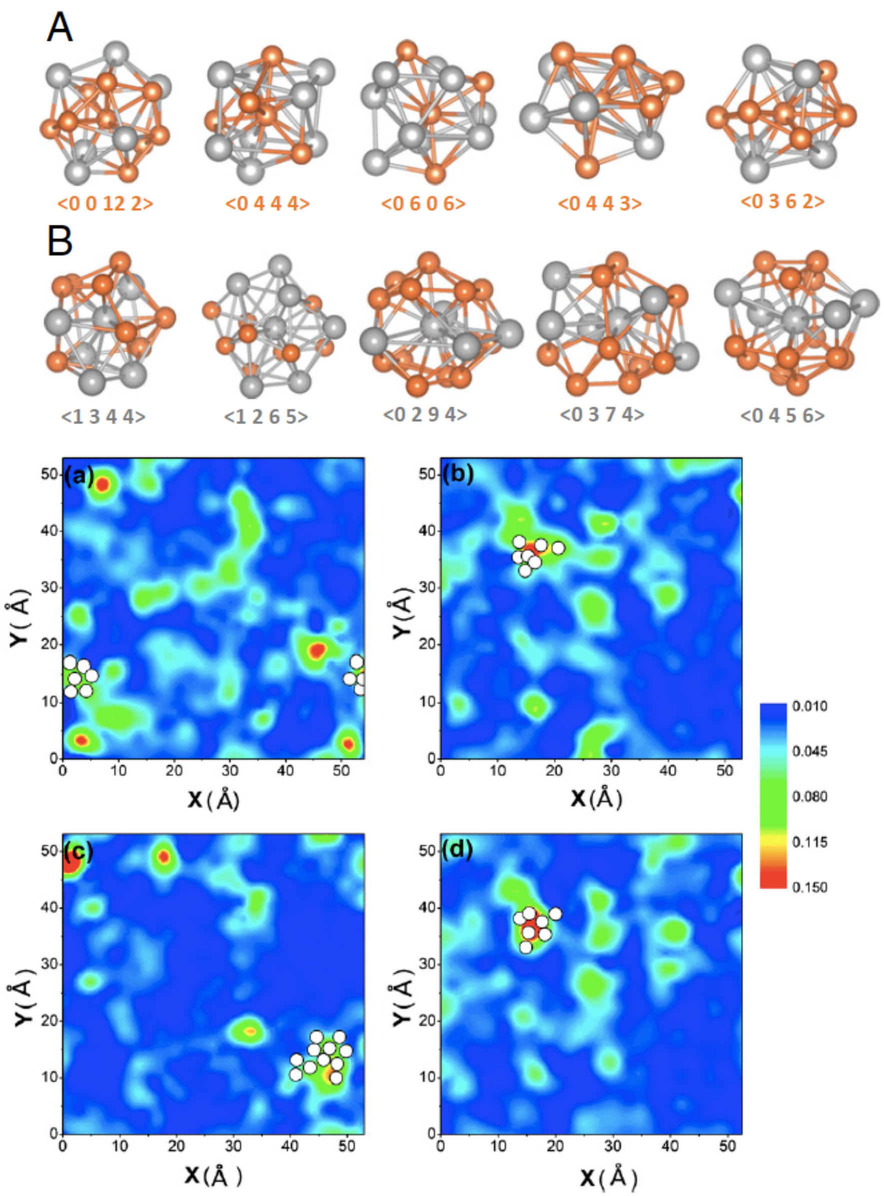
MANNING, LIU, PRL 107, 108302 (2011)

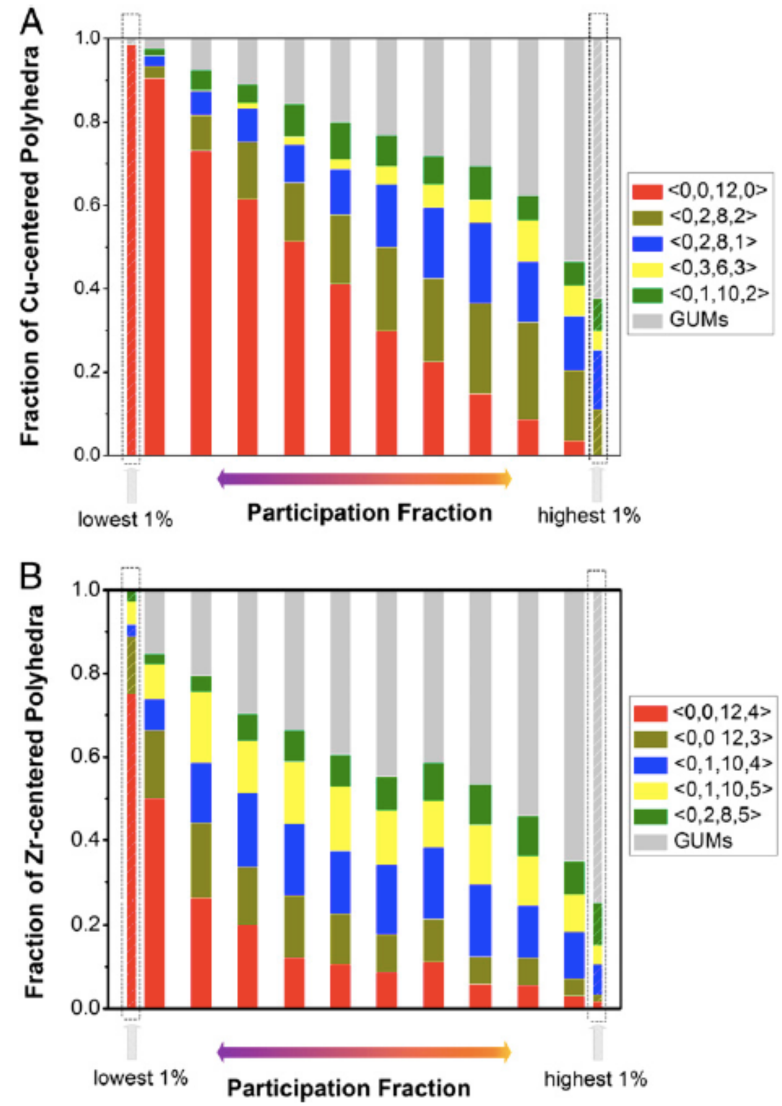
"Soft Spot" analysis of Manning and Liu



SOFT SPOTS AND THEIR STRUCTURAL SIGNATURE IN A METALLIC GLASS

DING, PATINET, FALK, CHENG AND MA, PNAS, V111, P14052 (2014)



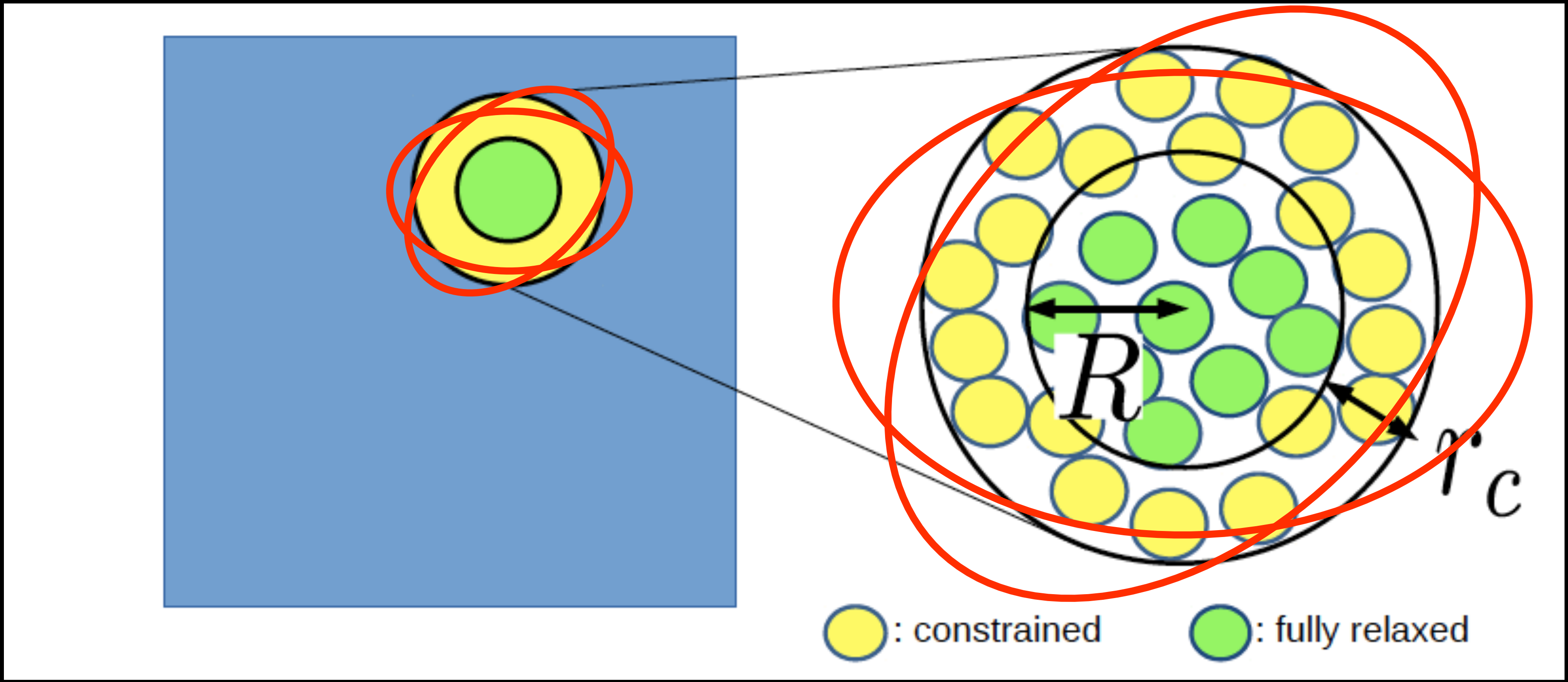


ANALYSIS OF LOCAL YIELD STRESS

PATINET, VANDEMBROUCQ AND FALK, PRL 117, 045501 (2016)

- Probe the local plastic rearrangement with local shear strain. Measure critical strain to instability.

- Originally proposed by P. Sollich as "Virtual strain method"
  Multiscale Modeling of Amorphous Solids Workshop, Dublin, Ireland (2011).



ANALYSIS OF LOCAL YIELD STRESS

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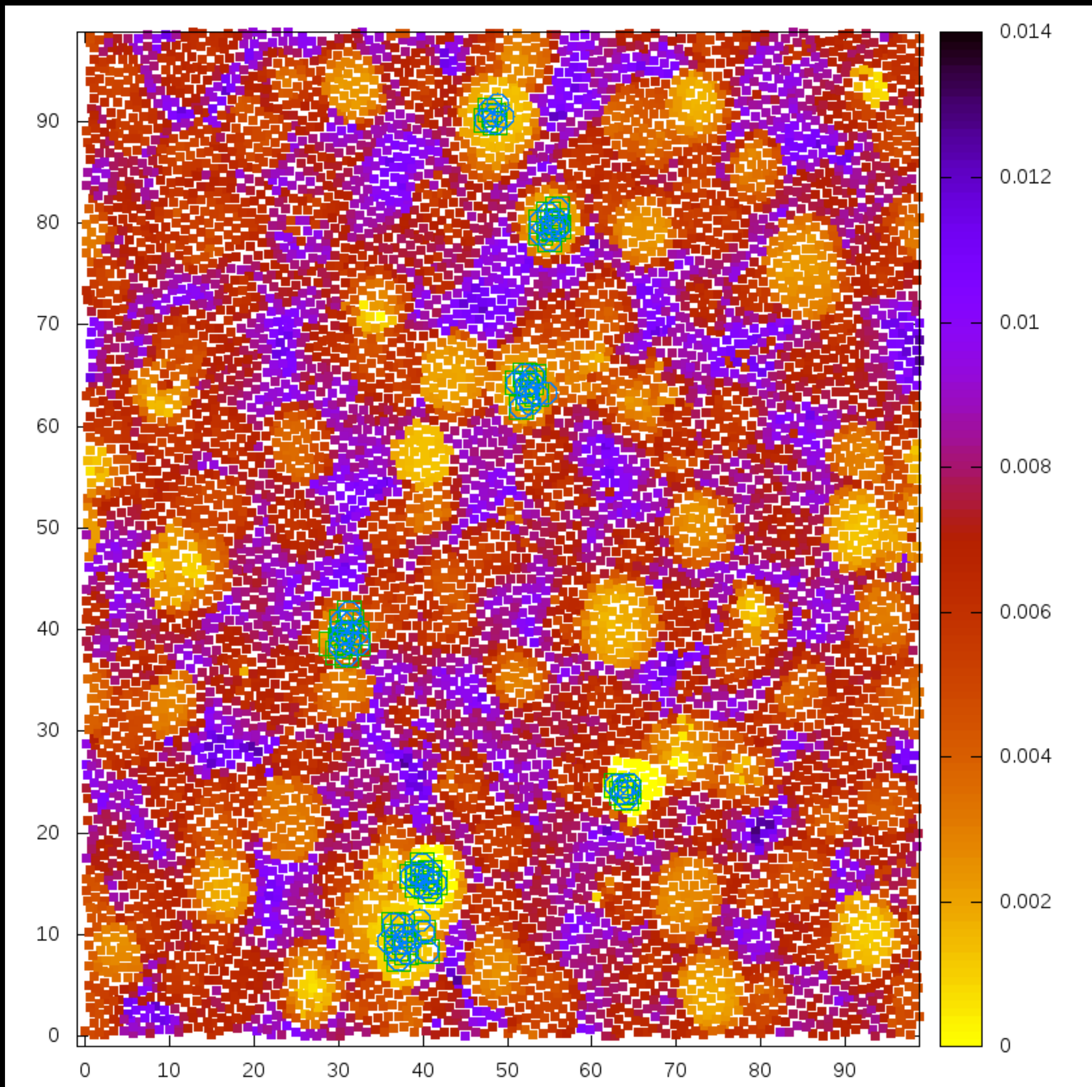
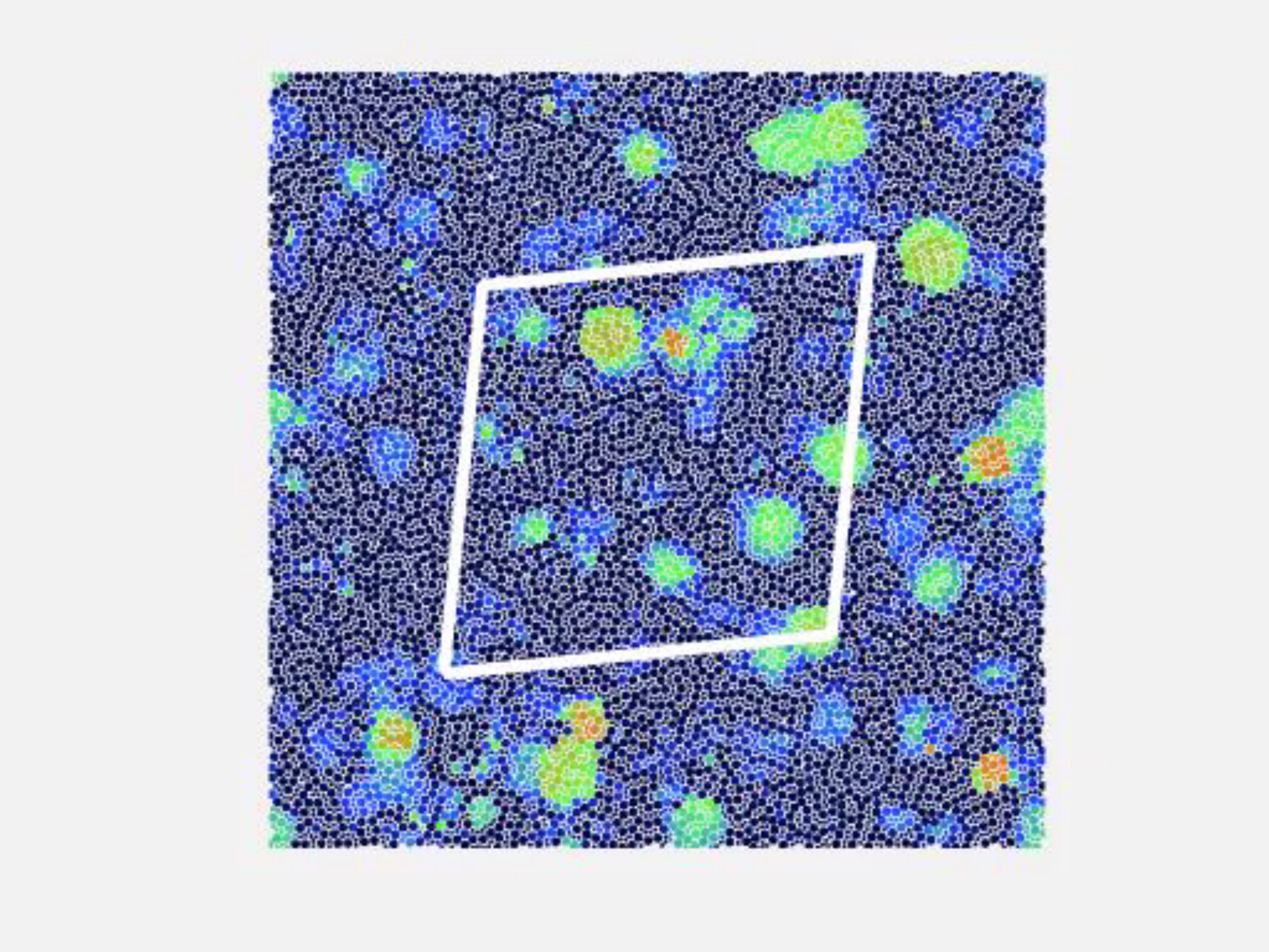


- 2D binary LJ system subjected to simple shear.
- Color shows minimum critical stress across 18 shear directions.
- Symbols show first event in each shear direction

Color map: $\min_{\theta} \; \sigma_c(\mathbf{x}, \theta)$ **Symbols:** center of plastic rearrangements

ANALYSIS OF LOCAL YIELD STRESS

PATINET, VANDEMBROUCQ, FALK, PRL 117, 045501 (2016)

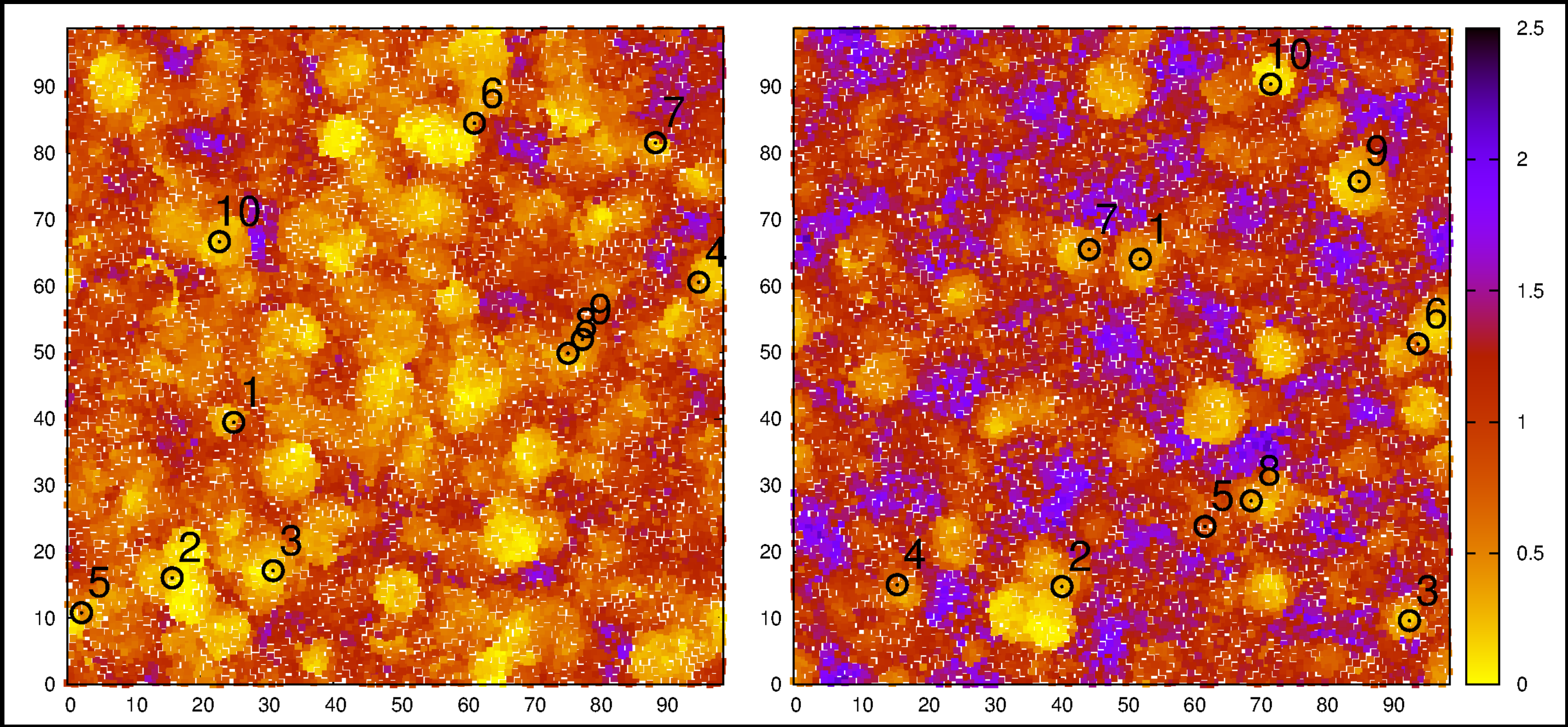


- Results are clearly **LOCAL** and **ORIENTATIONAL**

ANALYSIS OF LOCAL YIELD STRESS

PATINET, VANDEMBROUCQ AND FALK, PRL 117, 045501 (2016)

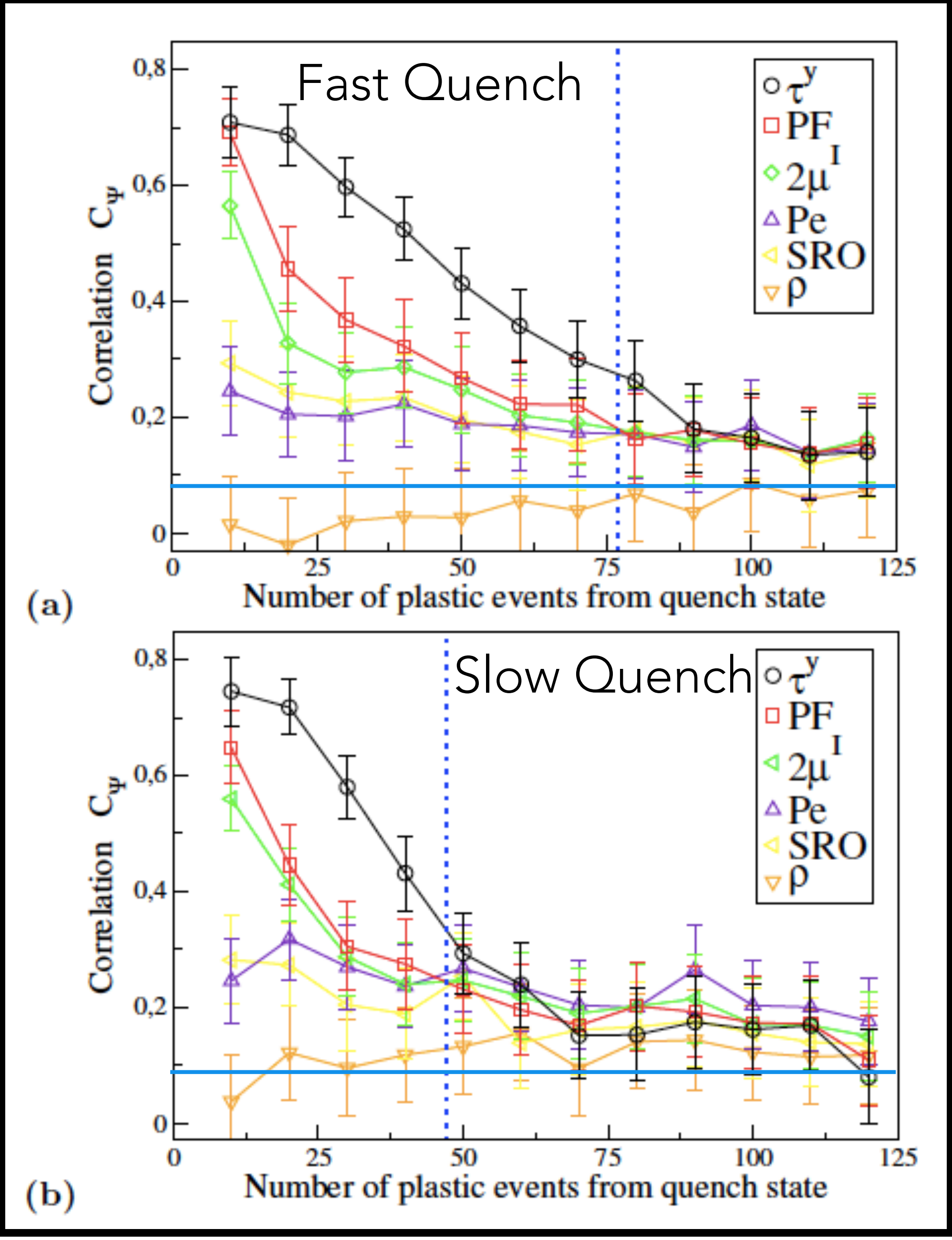
fast quench   slow quench



- Correlations **PERSIST** well past the first event
- Quench rate effects are evident

ANALYSIS OF LOCAL YIELD STRESS

PATINET, VANDEMBROUCQ AND FALK, PRL 117, 045501 (2016)



- Initial events equally well predicted by soft modes and virtual strain
- Subsequent events better predicted by virtual strain
- STZs persist for ~50 events
- Scales with # of events rather than %strain

STZ SUMMARY

- STZs exist and can be detected and characterized in atomistic simulation, but methods are still being developed, cross-compared and perfected.
- This puts us in a good position to ask how the STZ defect population evolves.
- We hope this will be helpful in evaluating hypotheses about what mesoscale structural parameters and theories are valuable (valid?) for thinking about microstructure evolution in amorphous solids.
- We must be careful however that in doing so we are distinguishing systems that may be governed by different physics.

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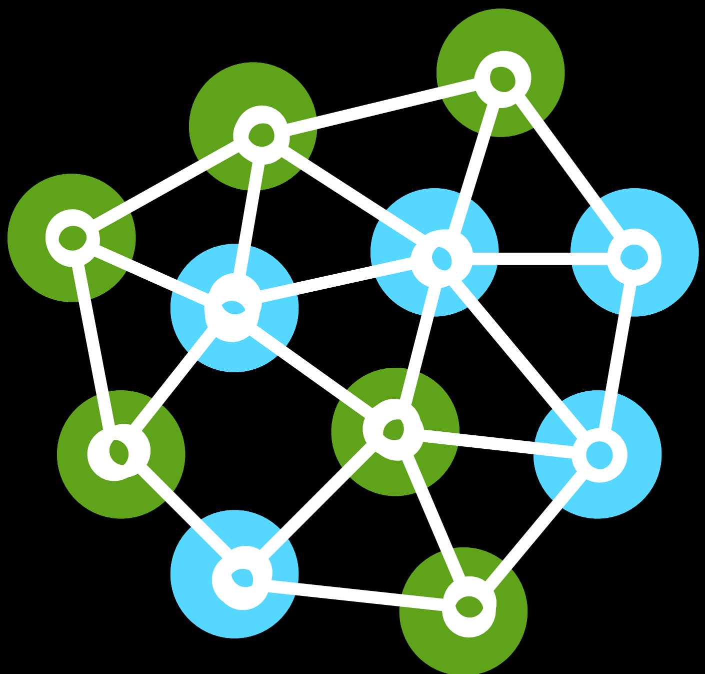
IS THERE A SCALAR QUANTITY THAT GOVERNS THE DEFECT DENSITY?

- **A number of such theoretical proposals/observations**
  - **Free Volume** (Turnbull and Cohen, Spaepen, Argon)
  - **Effective Temperature** (Falk, Langer, Bouchbinder) ***measured indirectly through average atomic potential energy***
  - **SP2/SP3 Bond Ratio in a-Si** (Demkowicz and Argon)
- **Do simulations and experiments of shear banding bear out these hypotheses?**
- **Are they perhaps inter-related? Which framework is most useful?**

A GLASS HAS TWO SUB-SYSTEMS

BOUCHBINDER, LANGER PRE, 80 031131,031132 (2009)



Fast Vibrational Sub-System

$$T \equiv \left(\frac{\partial U_R}{\partial S_R} \right)$$

Slow Configurational Sub-System

$$T_{eff} \equiv \left(\frac{\partial U_C}{\partial S_C} \right)_{\sigma, \{\Lambda\}}$$

RELATING ATOMIC POTENTIAL ENERGY TO THE EFFECTIVE TEMPERATURE

- Analogy with specific heat for fast degrees of freedom

$$C = \frac{\partial U_R}{\partial T} \to C\,\Delta T \approx \Delta U_R$$

$$C_{eff} = \frac{\partial U_C}{\partial T_{eff}} \to C_{eff}\,\Delta T_{eff} \approx \Delta U_C$$

- We calculate **χ** assuming a linear relationship

$$\chi \equiv \frac{k_B\,T_{eff}}{e_Z} \approx \frac{k_B}{e_Z\,C_{eff}}(U_C - U_0) \equiv \beta\,(U_C - U_0)$$

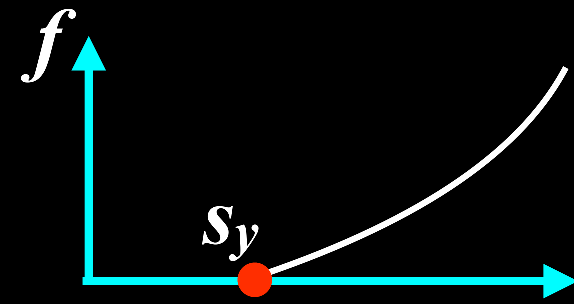
- From c we infer the defect density of STZs

$$\rho_{STZ} \propto \exp\left(-1/\chi\right)$$

STZ CONSTITUTIVE THEORY

BOUCHBINDER, LANGER PRE, 80 031131,031132 (2009)

Number of defects is proportional to **exp(-1/χ)**



$$\dot{\epsilon}^{pl}_{ij} = \exp\left(-1/\chi\right)\ f_{ij}\left(s_{kl}\right)$$

$$c_0\dot{\chi} = s_{ij}\dot{\epsilon}^{pl}_{ij}\left(\chi_\infty - \chi\right) + \nabla\cdot\left(l^2\left|\dot{\epsilon}^{pl}\right|\nabla\chi\right)$$

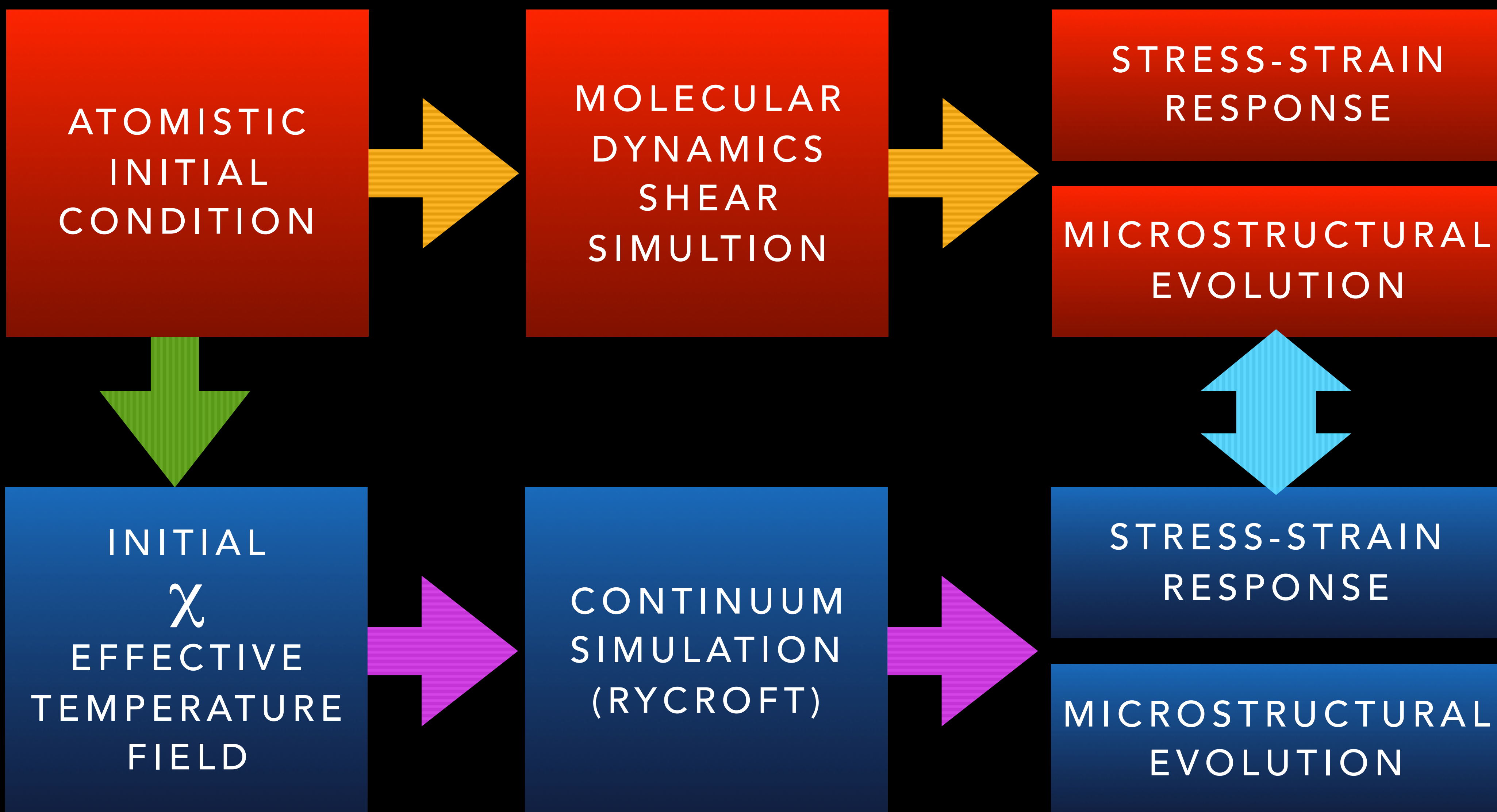
Transformation rate f depends on applied shear stress and is zero below a yield stress s_y

Rate of increase of effective temperature χ is proportional to rate of plastic work

Gradient term that describes diffusion of the effective temperature χ.

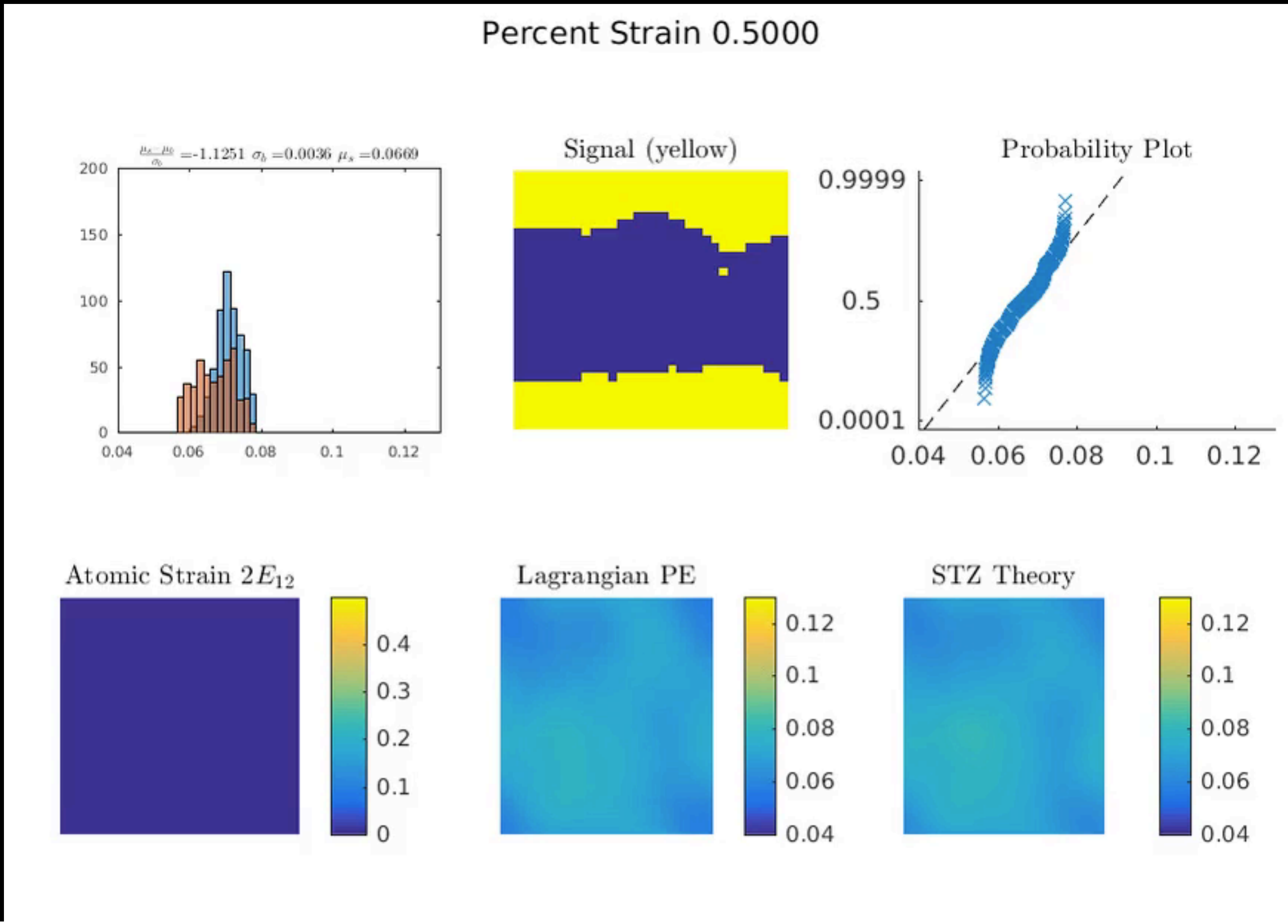
DIRECTLY CONNECTING MD SIMULATION AND CONTINUUM THEORY

HINKLE, RYCROFT, SHIELDS AND MLF, PRE, 95, 053001 (2017)



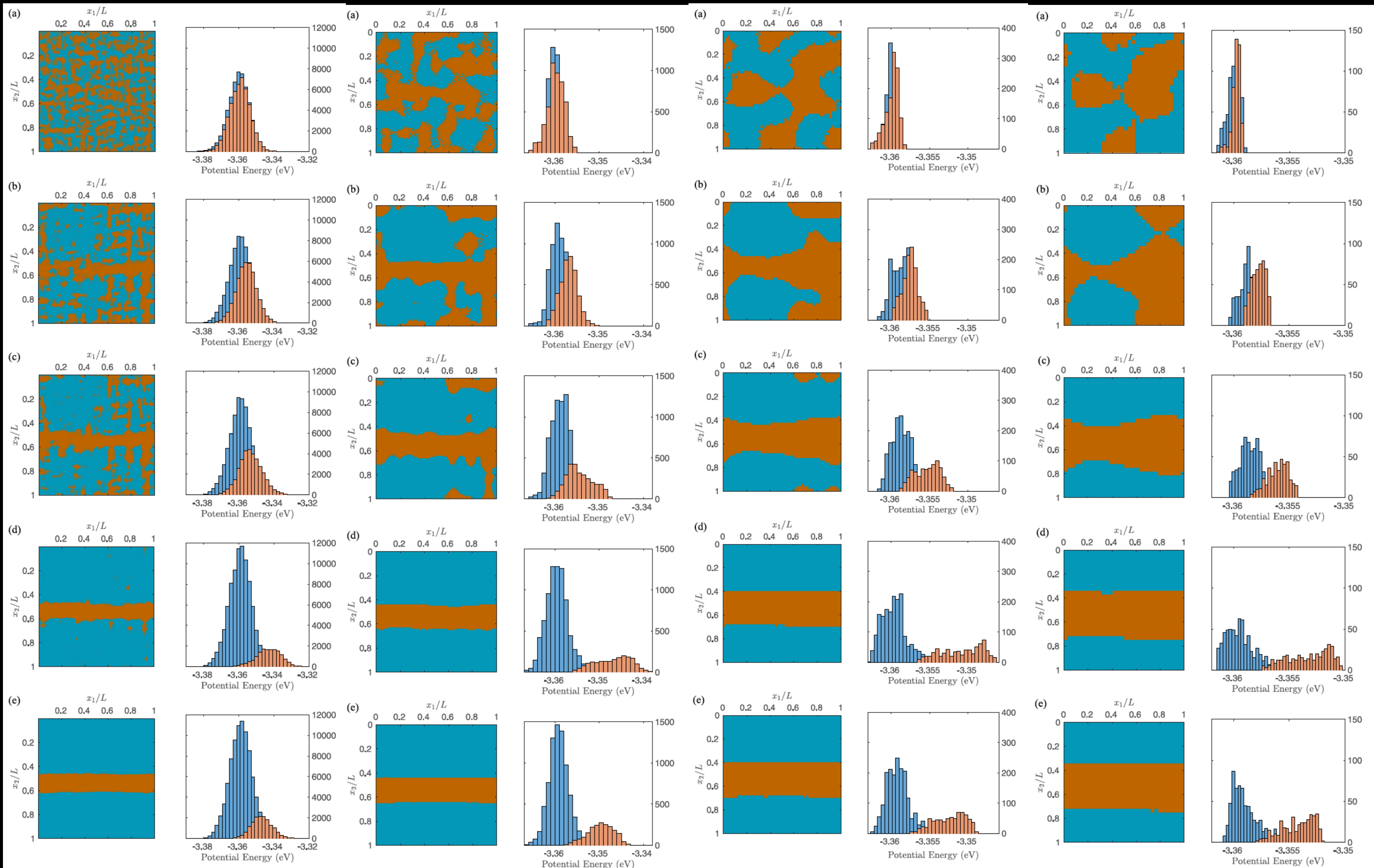
ATOMISTICALLY INFORMED CONTINUUM MODELING OF CuZr ALLOYS

HINKLE, RYCROFT, SHIELDS AND MLF, PRE, 95, 053001 (2017)



STRAIN COARSE GRAINING

5Å 16Å 32Å 50Å



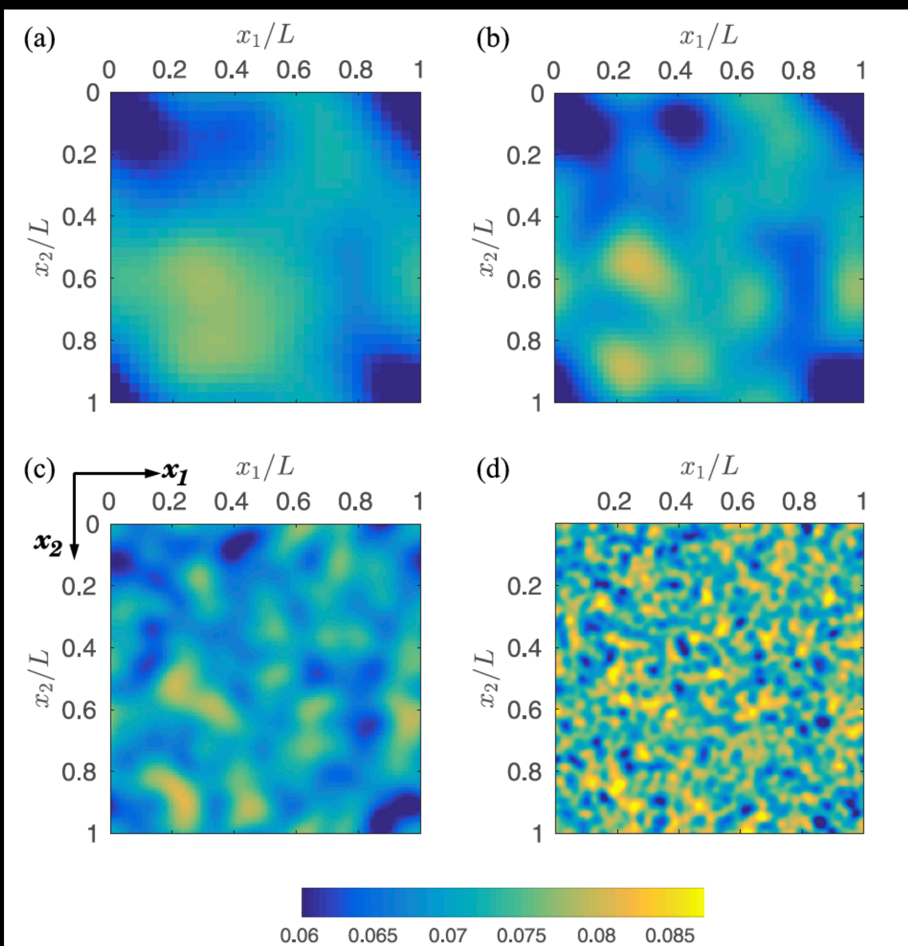
HINKLE, RYCROFT, SHIELDS AND MLF, PRE, 95, 053001 (2017)

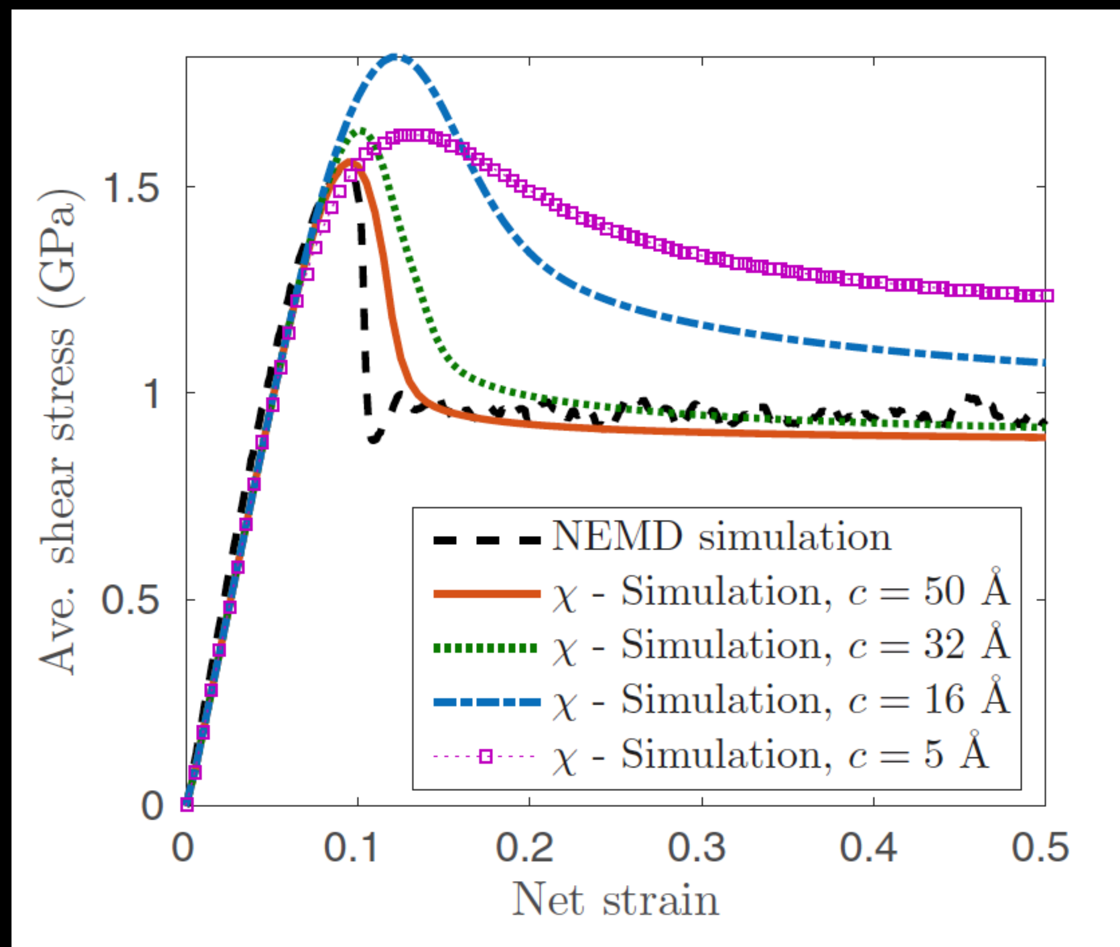
POT. ENERGY COARSE GRAINING

HINKLE, RYCROFT, SHIELDS AND MLF, PRE, 95, 053001 (2017)

PARAMETERS		UNIT	Value
Yield stress	s_y	GPa	0.85
STZ size	ϵ_0	—	10
Inverse attempt frequency	τ_0	ps	0.1
Elastic shear modulus	μ	GPa	20
Plastic-work fraction	c_0	—	0.3
Global shear rate	$\dot{\gamma}$	ps^{-1}	10^{-4}
Diffusivity length	l	Å	4.01

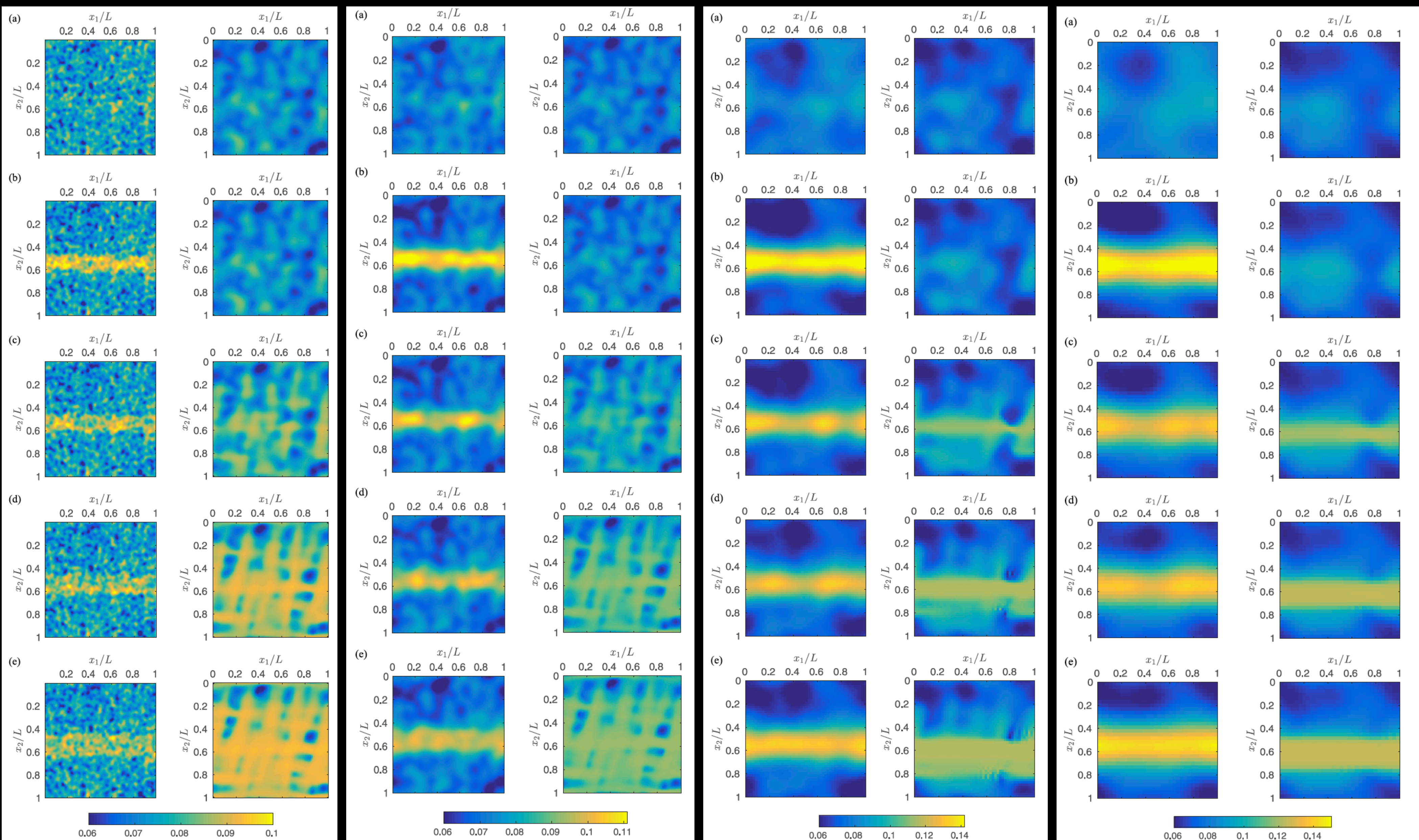
c (Å)	β	E^o (eV)	χ_∞
50	9.5	−3.367	0.13
32	6.1	−3.371	0.12
16	2.3	−3.390	0.094
5	0.92	−3.440	0.085





POT. ENERGY COARSE GRAINING / CONTINUUM MODELING

5Å 16Å 32Å 50Å



HINKLE, RYCROFT, SHIELDS AND MLF, PRE, 95, 053001 (2017)

EFFECTIVE TEMPERATURE SUMMARY

- Reasonable **cross-comparisons** can be made between the **Effective Temperature STZ Theory** and molecular dynamics (**MD**) simulations with proper parameterization.
- One important factor beyond the constitutive model itself is the scale of **coarse-graining**, which must be sufficiently large for reasonable comparisons to result.
- **Open questions** remain about how the parameters of the model are effected by changes in **processing** (quench rate) and **alloy composition**.

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