RIGIDITY OF SOLIDS:
a thermodynamic origin story

Surajit Sengupta (TCIS)

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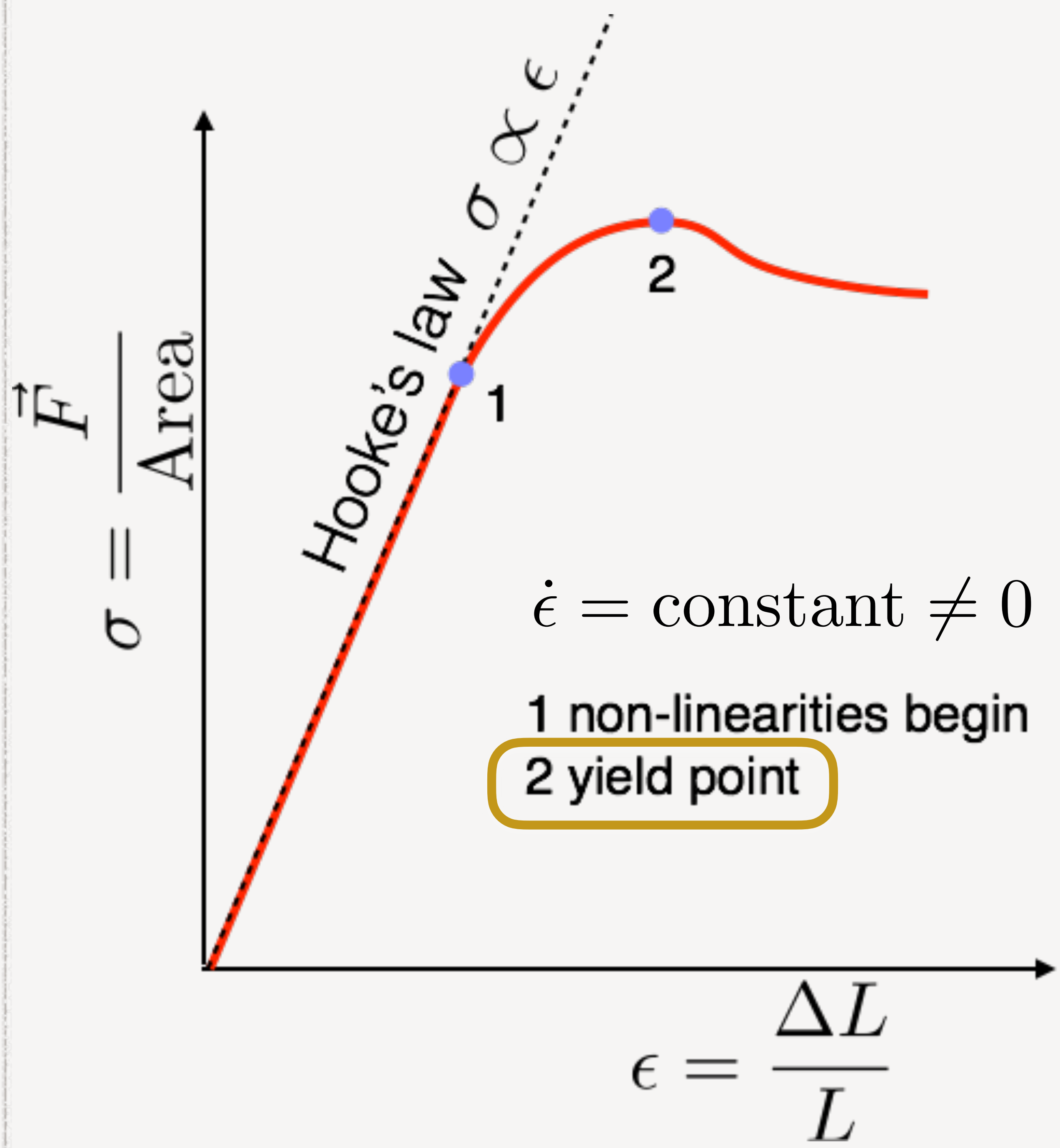
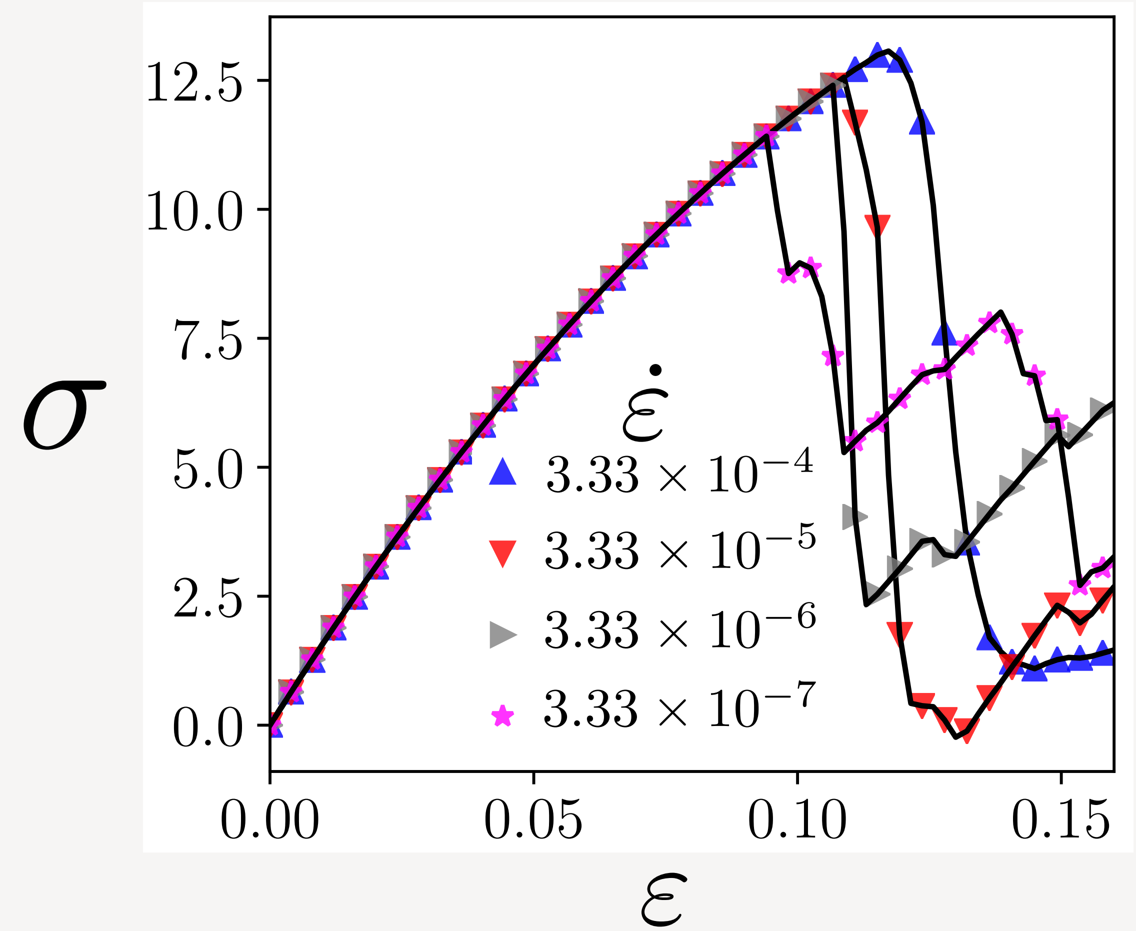
STATING THE PROBLEM:





MD simulations of a 2d LJ (triangular) solid, which is *initially* defect free, under pure shear.

What leads to loss of rigidity and onset of plasticity in a crystalline solid?

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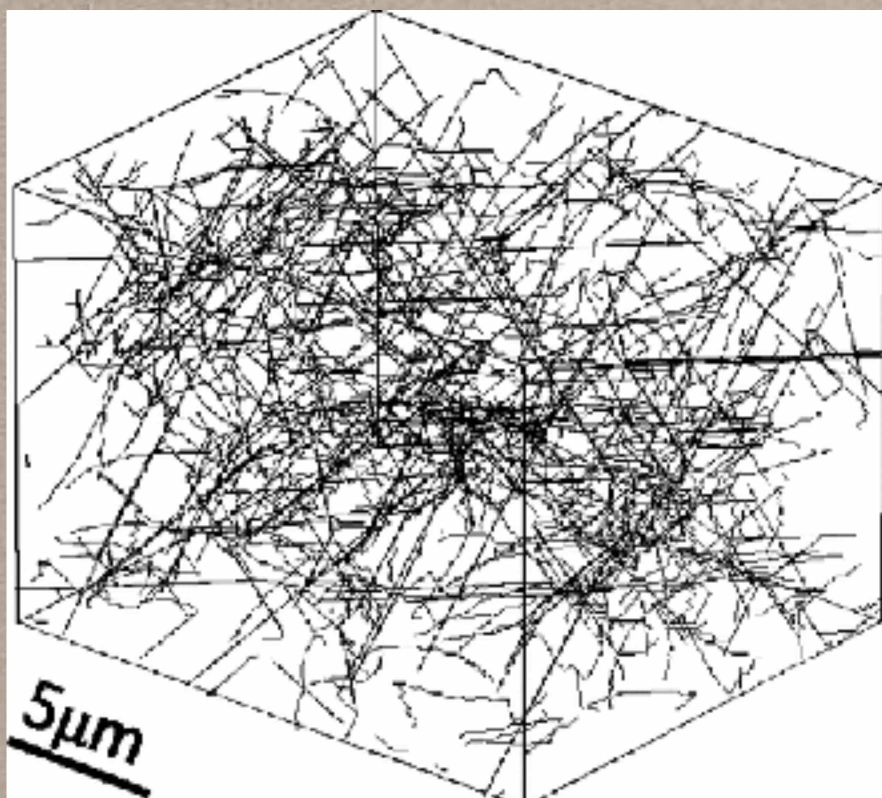
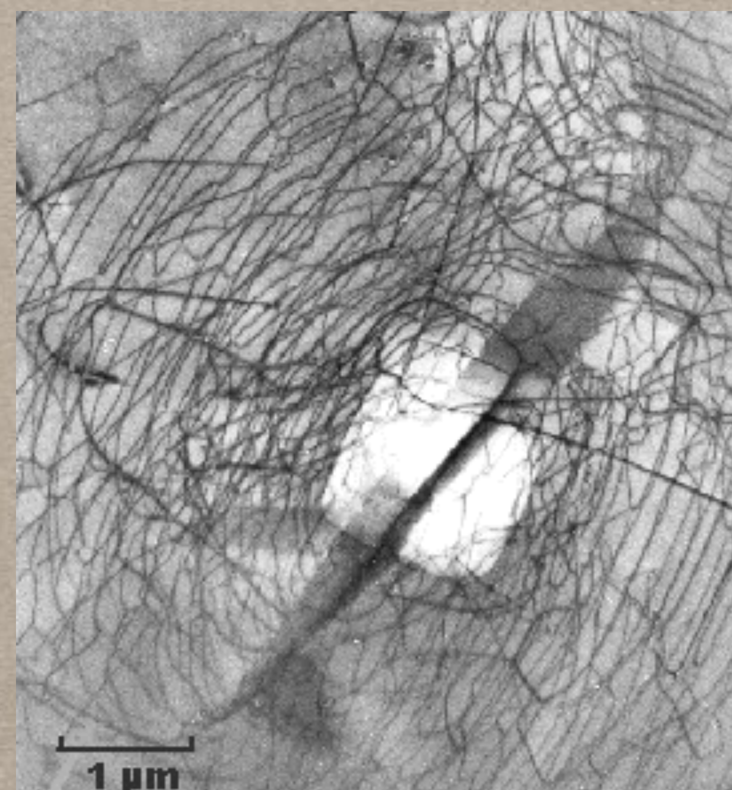
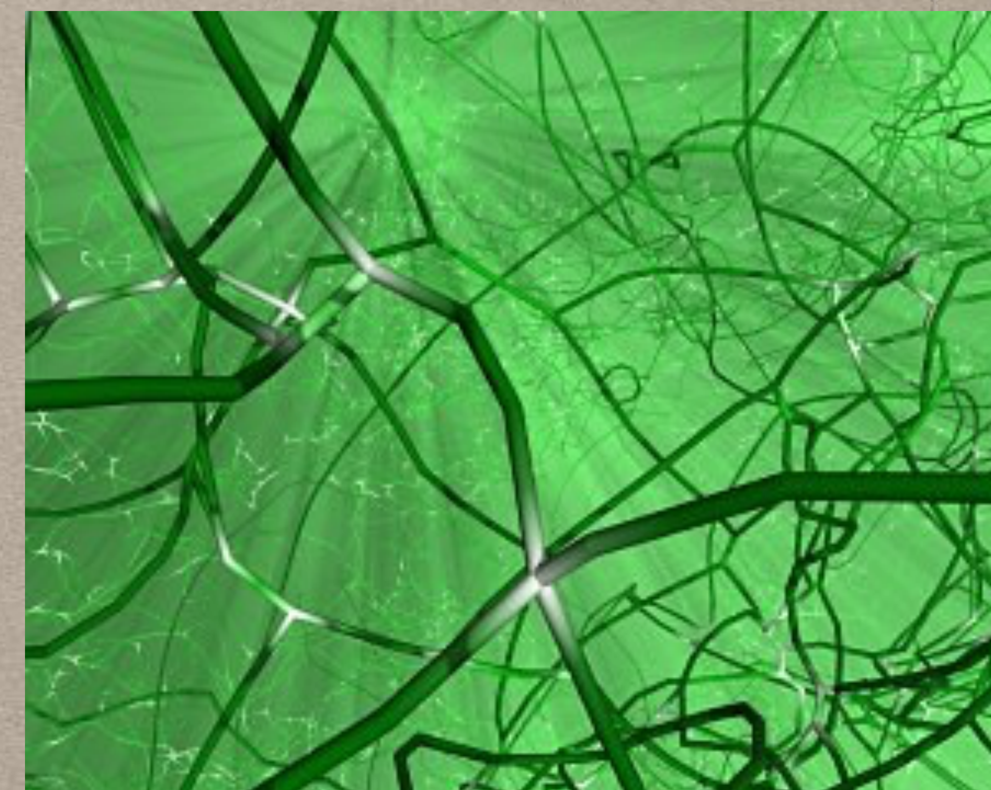
Crystalline solids are rigid but loose this property at some fixed (large) stress value - the so called yield stress - due to nucleation and dynamic de-pinning/un-jamming of dislocations.







V. Bulatov et al., Nature (2006); M. Marder, Les Houches Lectures

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THEORIES OF YIELDING

PRL **102,** 175501 (2009) PHYSICAL REVIEW LETTERS week ending 1 MAY 2009

Micromechanical Model for Deformation in Solids with Universal Predictions for Stress-Strain Curves and Slip Avalanches

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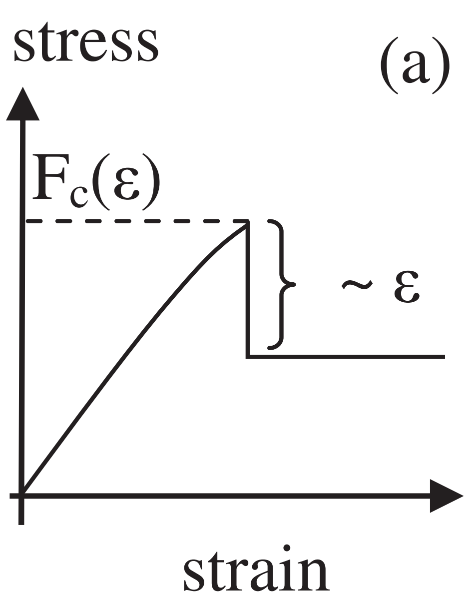
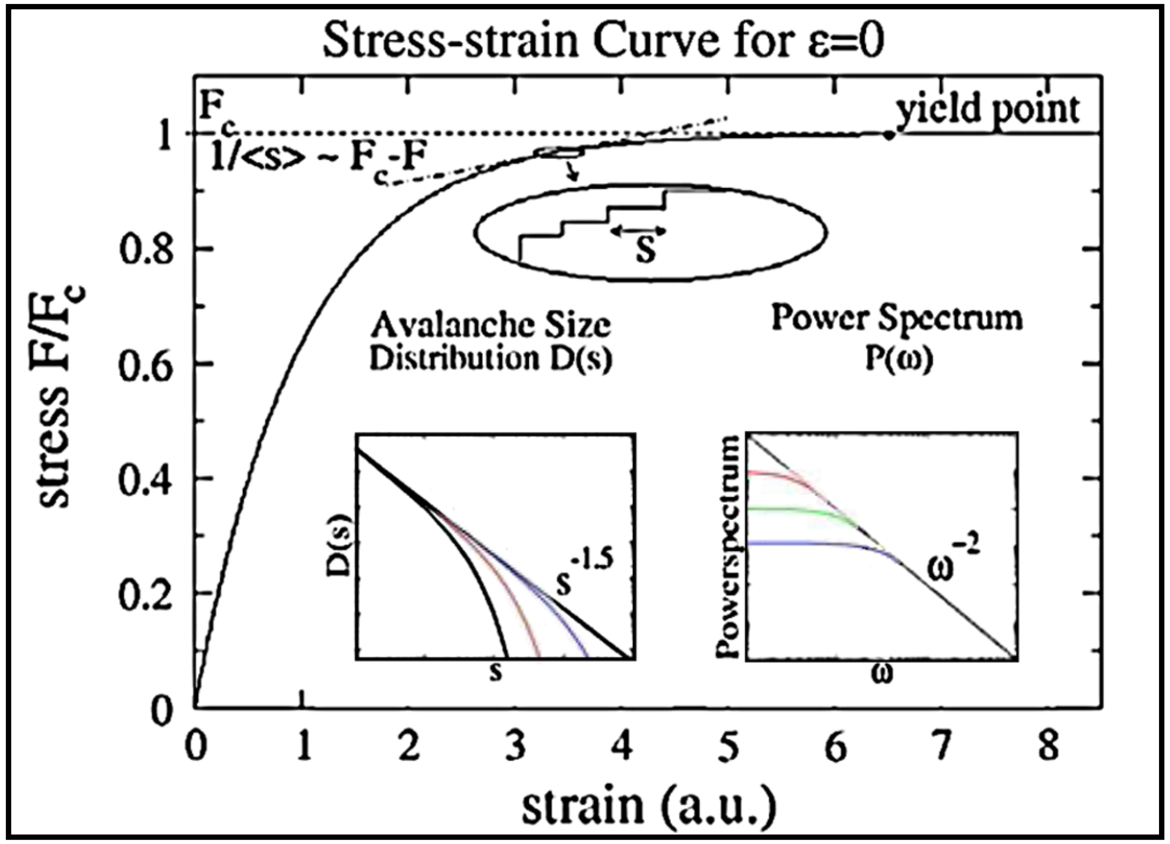
(Received 23 May 2008; published 27 April 2009)



EPL, **101** (2013) 36003
doi: 10.1209/0295-5075/101/36003



Determination of the universality class of crystal plasticity

G. Tsekenis, J. T. Uhl, N. Goldenfeld and K. A. Dahmen

Department of Physics, University of Illinois at Urbana-Champaign, Loomis Laboratory of Physics 1110 West Green Street, Urbana, IL, 61801-3080, USA

- N elastically connected elements
- Starting from zero stress external stress is increased till system undergoes a de-pinning transition
- When local stress exceeds a threshold stress is reset to zero locally
- Stress is redistributed, which may cause avalanches
- Avalanches show power law distribution with “interface de-pinning” exponents
- Can explain some experimental phenomenology
- Not a microscopic theory ! Yielding (output) is incorporated in the stress thresholds (input)

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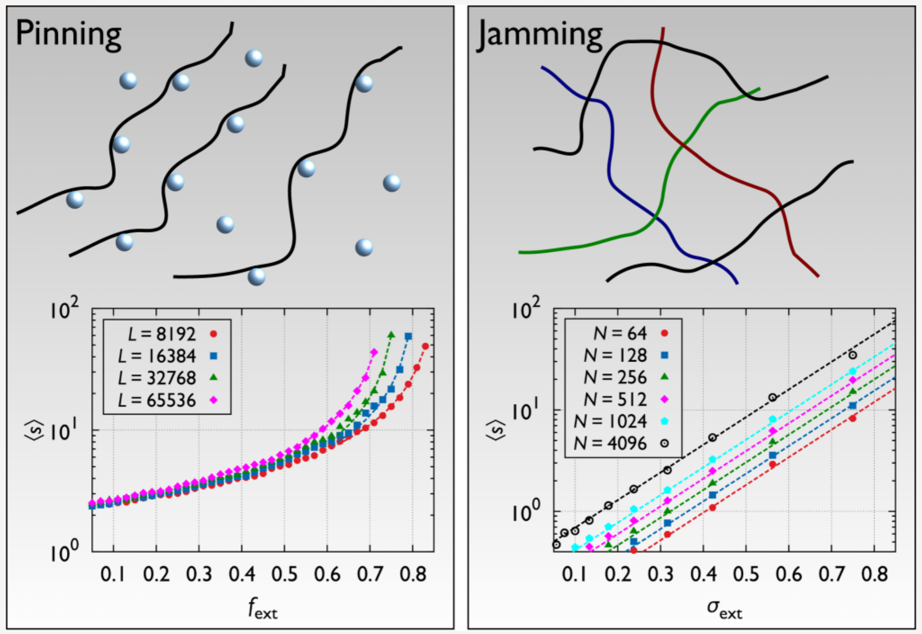
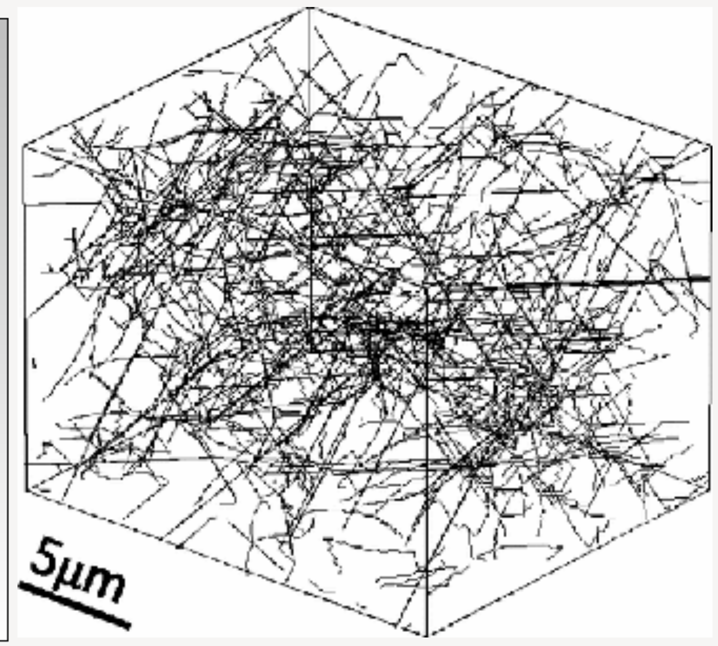
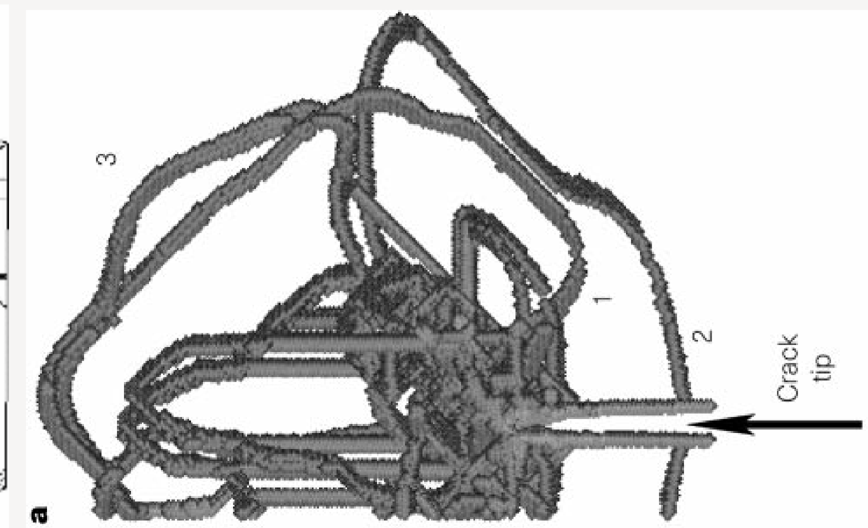
PRL 112, 235501 (2014) PHYSICAL REVIEW LETTERS week ending 13 JUNE 2014

Avalanches in 2D Dislocation Systems: Plastic Yielding Is Not Depinning

Péter Dusán Ispánovity,[1,*] Lasse Laurson,[2] Michael Zaiser,[3] István Groma,[1] Stefano Zapperi,[4] and Mikko J. Alava[2]







letters to nature

Connecting atomistic and mesoscale simulations of crystal plasticity

Vasily Bulatov*, Farid F. Abraham†, Ladislas Kubin‡, Benoit Devincre‡ & Sidney Yip*

VOLUME 89, NUMBER 25 PHYSICAL REVIEW LETTERS 16 DECEMBER 2002

From Dislocation Junctions to Forest Hardening

R. Madec, B. Devincre, and L. P. Kubin

A quantitative description of plastic deformation in crystalline solids requires a knowledge of how an assembly of dislocations—the defects responsible for crystal plasticity—evolves under stress[1]. In this context, molecular-dynamics simulations ...

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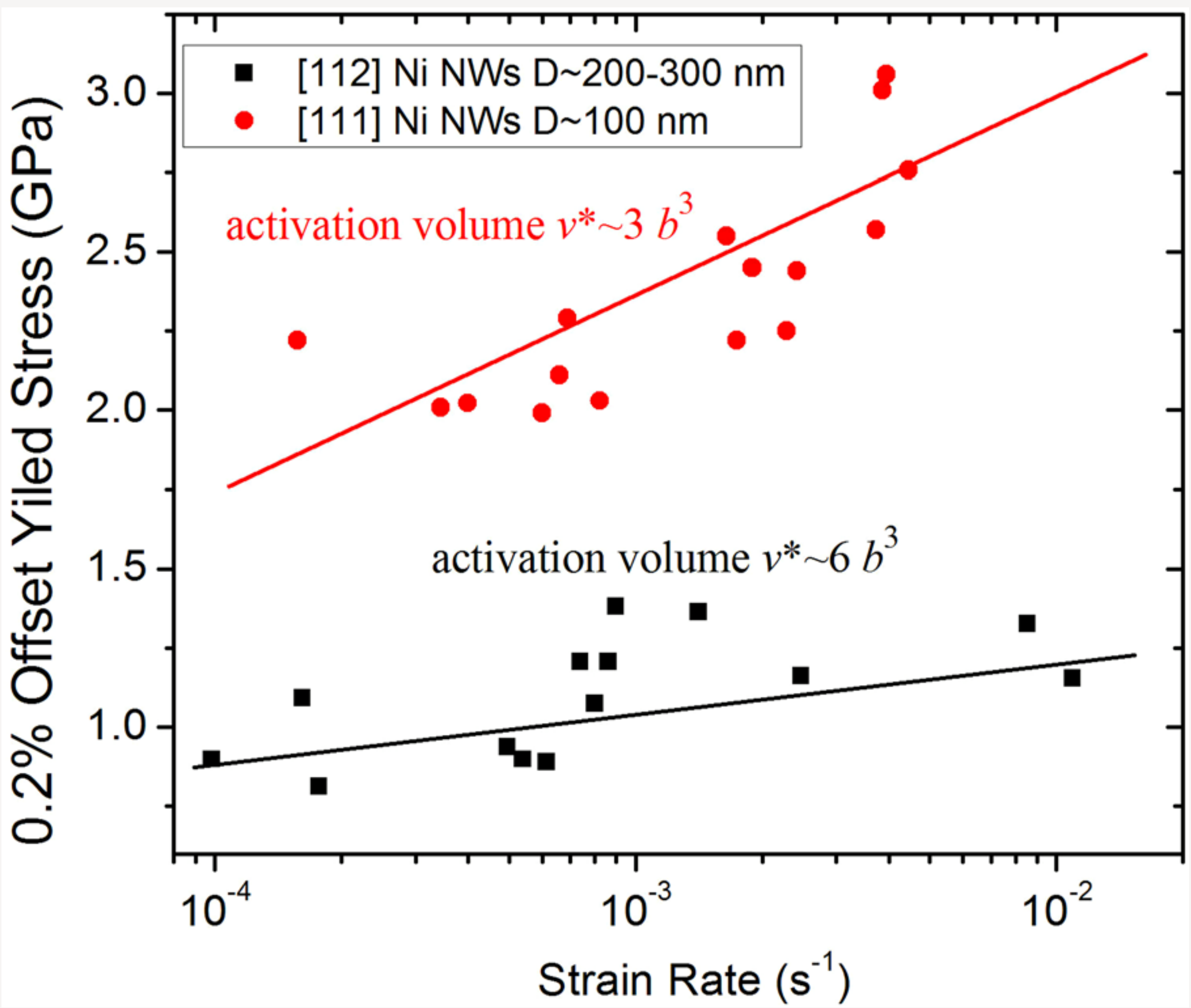
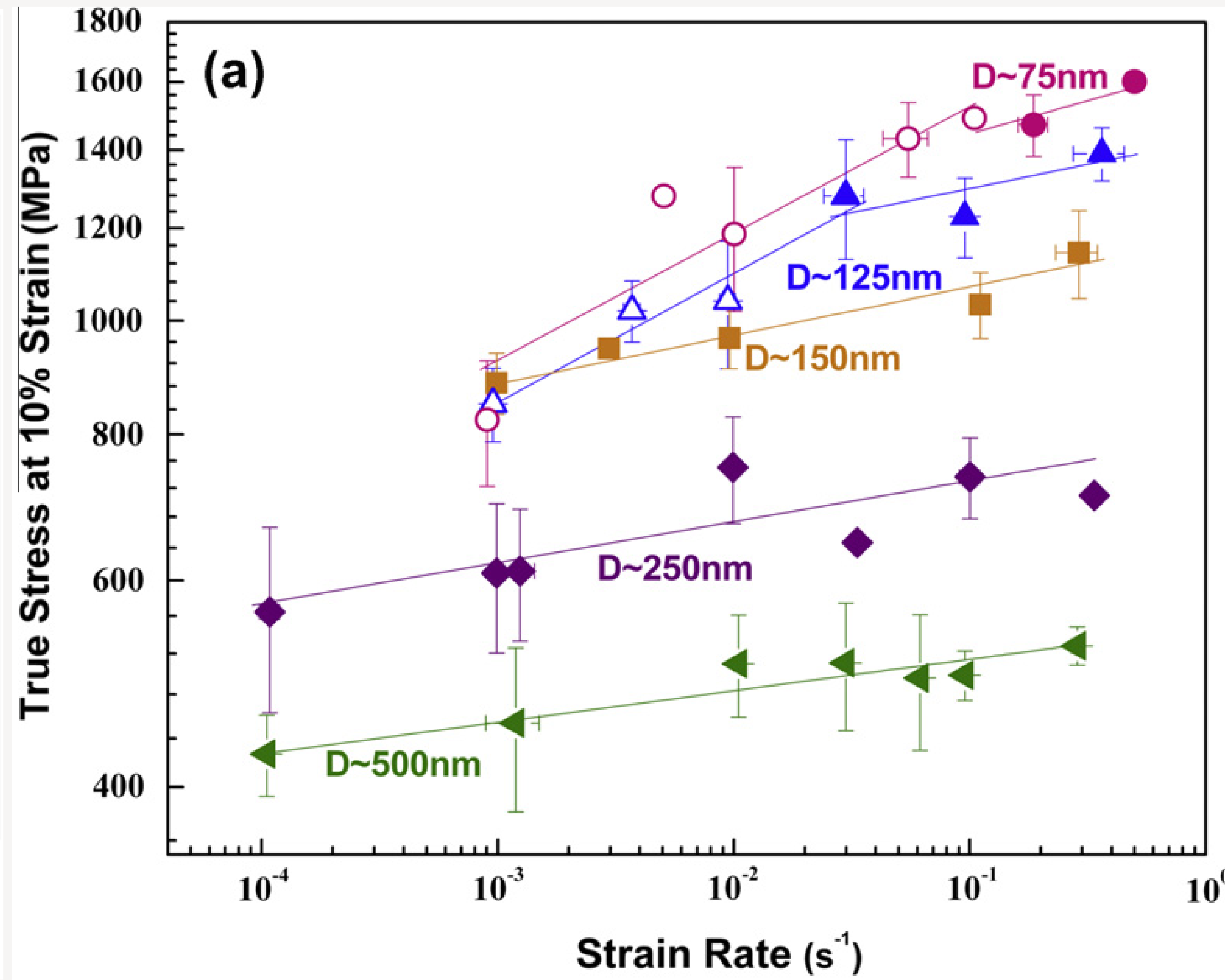
STRAIN RATE SENSITIVITY
AND
CREEP?

STRAIN RATE SENSITIVITY

Ni nano-wires

Cu nano-pillars



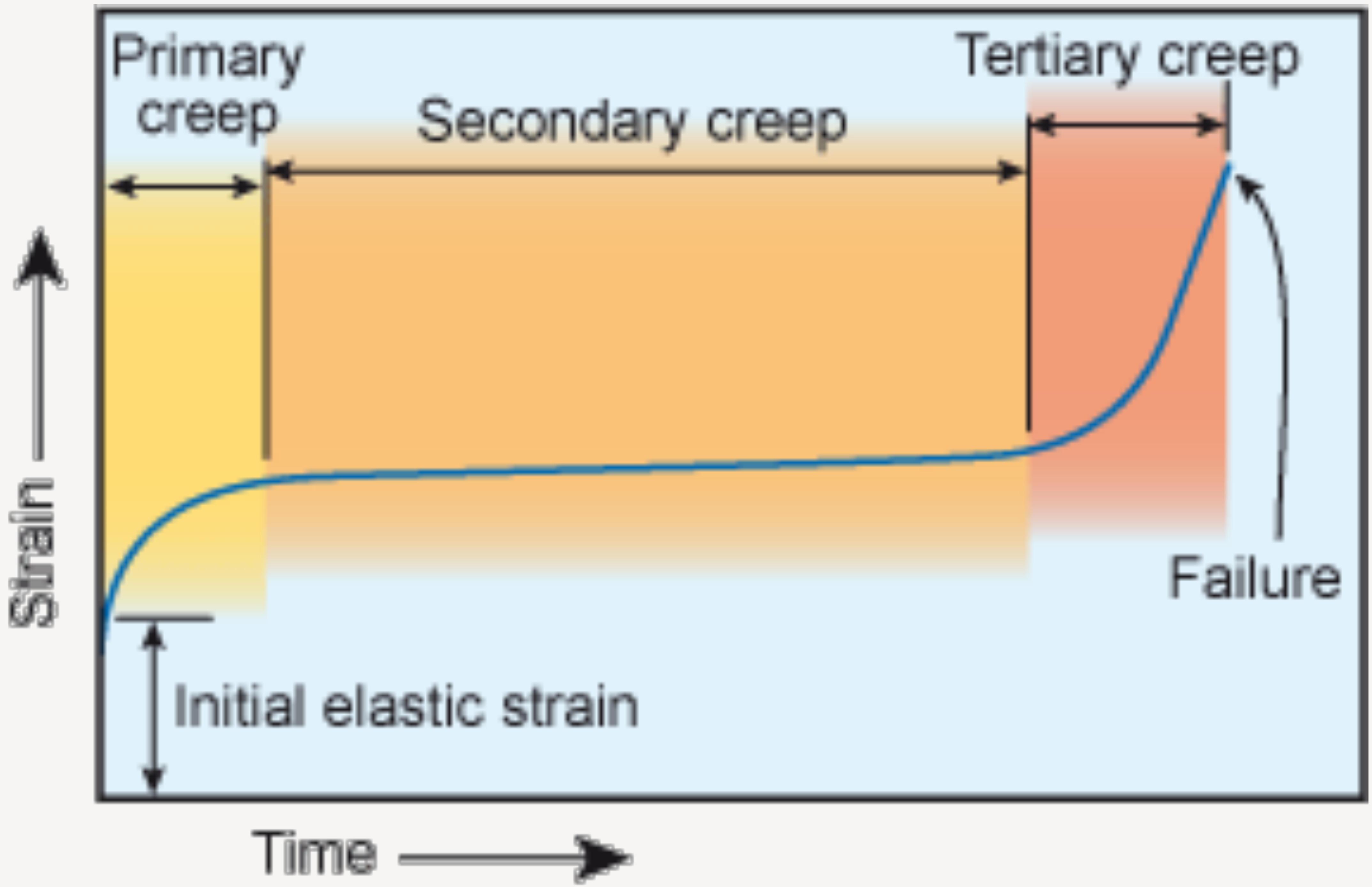


Peng et al. *Appl. Phys. Lett.* **102**, 083102 (2013)

Jennings et al. *Acta Mat.* **59**, 5 1)

$$\sigma = \sigma_0 \dot{\varepsilon}^m \qquad 0.03 \lesssim m \lesssim 0.06$$

CREEP


Primary creep
Secondary creep
Tertiary creep
Strain
Failure
Initial elastic strain
Time

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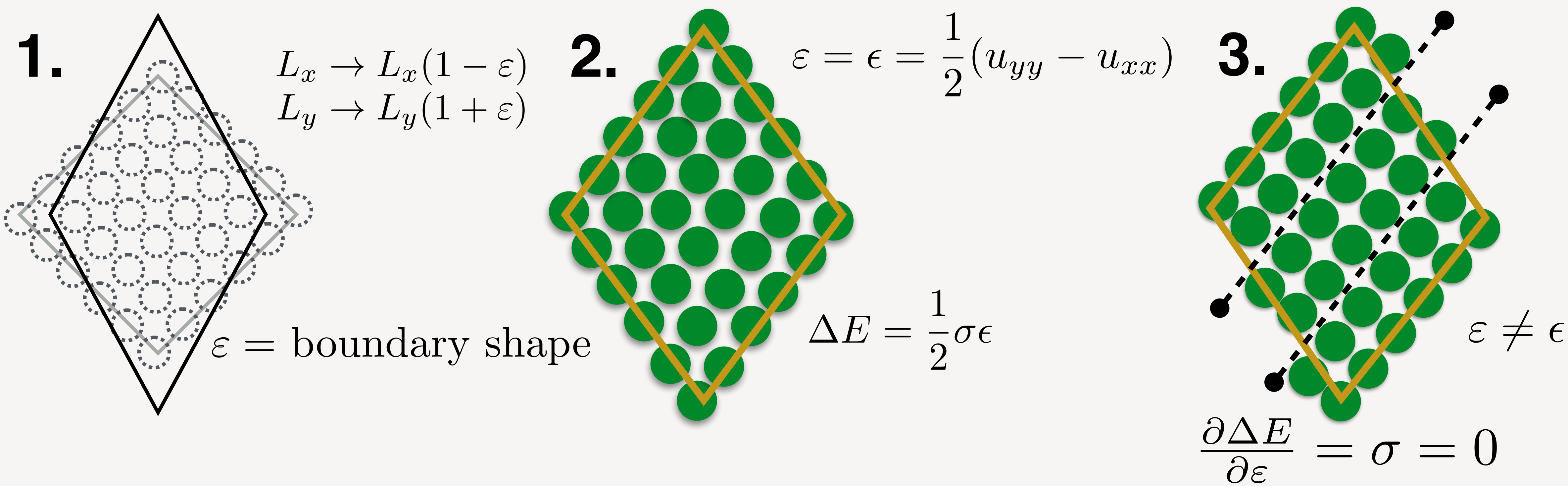
Equilibrium, *bulk,* free energy is independent of the shape of the boundary

D. Ruelle, *Statistical Mechanics: Rigorous Results* (Benjamin, New York, 1969).



Non-zero stress only from constrained minimisation

O. Penrose, Markov Processes Relat. Fields **8**, 351 (2002).
S. Shaw and P. Harrowell, Phys. Rev. Lett. **116**, 137801 (2016)

Or a finite time average:

F. Sausset, G. Biroli, and J. Kurchan, J. Stat. Phys. **140**, 718 (2010).
R. Bruinsma, B. I. Halperin and A. Zippelius Phys. Rev. B **25**, 579 (1982)

OUTLINE

- First-order phase transitions
- Affine and *non affine* atomic displacements: a new collective variable for plastic deformation.
- Rigidity: consequence of an "*invisible*" first order phase transition involving non-affine displacements
- Yielding as the *visible, dynamic* consequence of this transition
- Can understand *initiation* of plasticity in an *initially ideal crystal* without invoking properties of dislocations! (Remember: no dislocations in glasses)

Nath et al. Proc. Natl. Acad. Sci. USA (2018)

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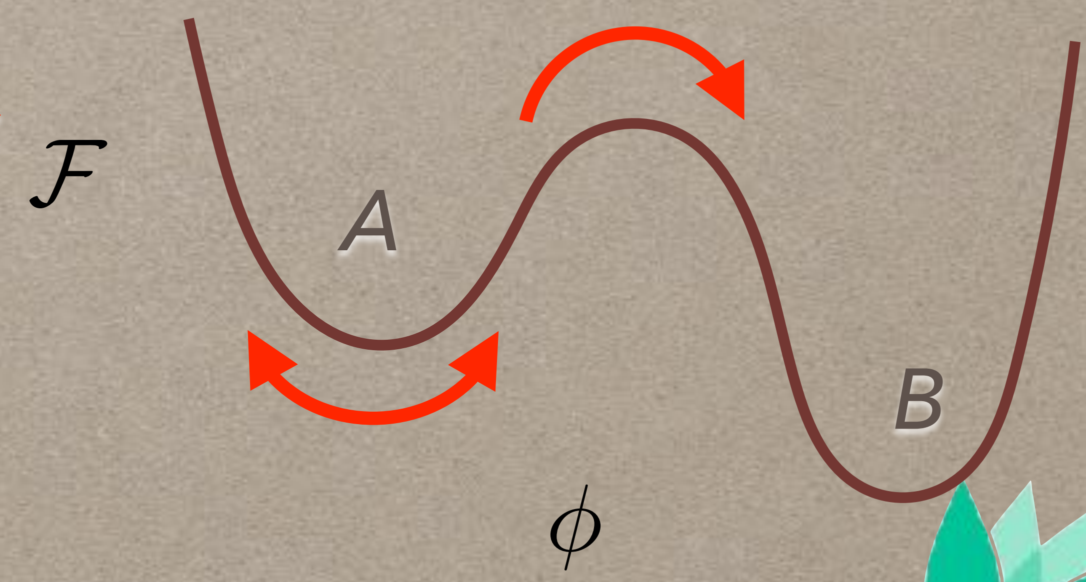
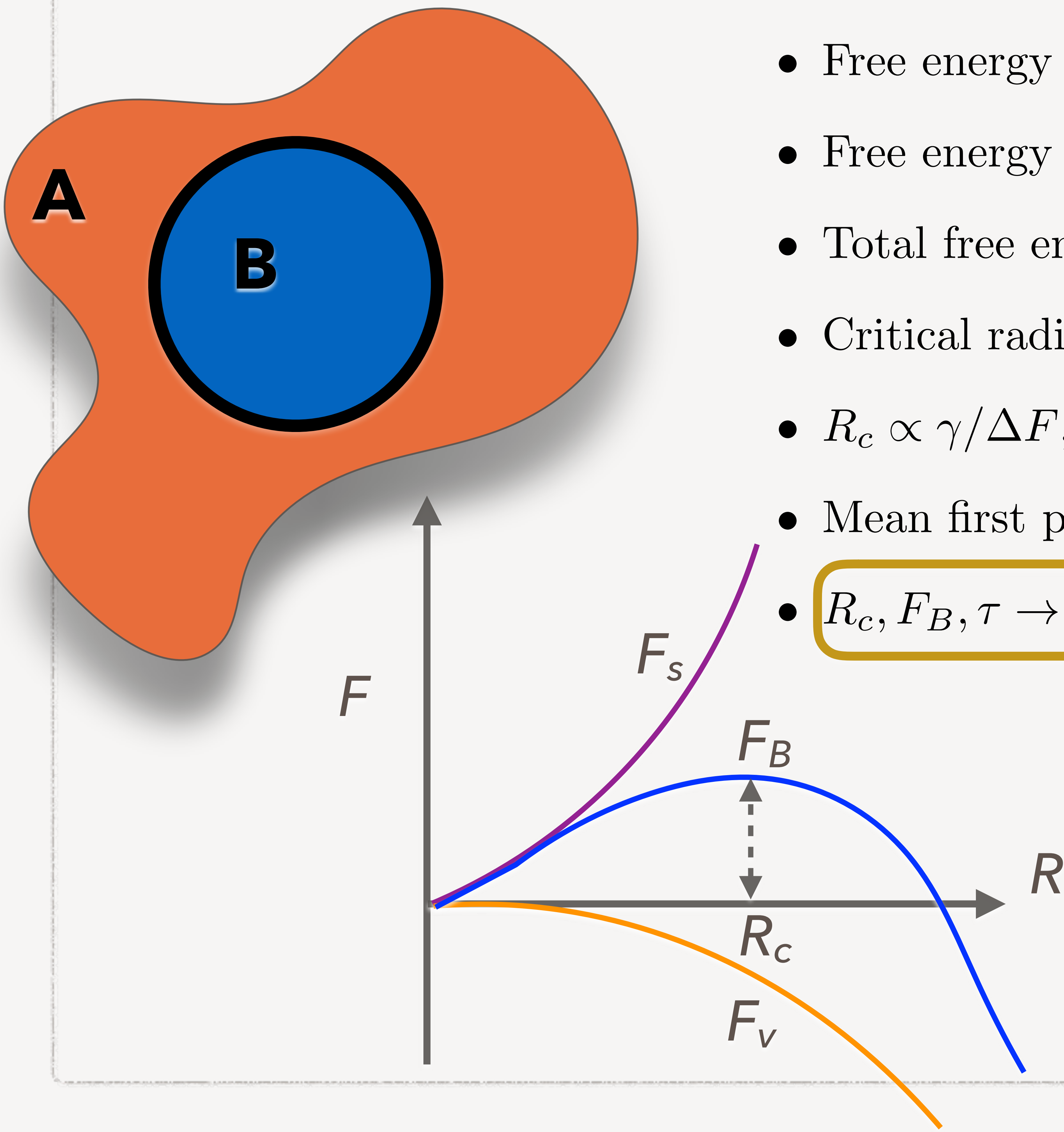
FIRST ORDER TRANSITION

- Sharp ***discontinuous*** changes; latent heat
- Phase ***coexistence*** for choice of external parameters
- Presence of an ***interface*** separating coexisting phases
- ***Metastability*** and ***hysteresis***



CLASSICAL NUCLEATION THEORY



- Free energy gain $F_V = \Delta F \quad \frac{4}{3}\pi R^3$
- Free energy cost $F_S = \gamma \quad 4\pi R^2$
- Total free energy $F = F_V + F_S$
- Critical radius R_c and free energy barrier F_B
- $R_c \propto \gamma/\Delta F$, $F_B \propto \gamma^3/\Delta F^2$
- Mean first passage time $\tau = \tau_0 e^{\beta F_B}$
- $\boxed{R_c, F_B, \tau \to \infty \text{ as } \Delta F \to 0.}$

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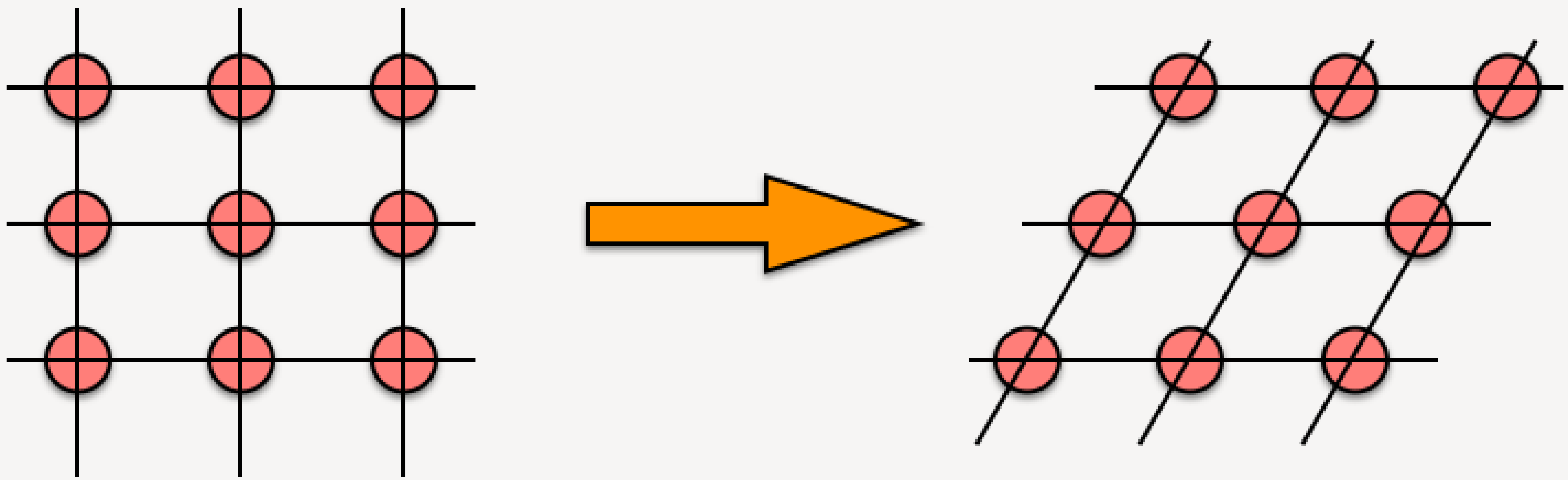
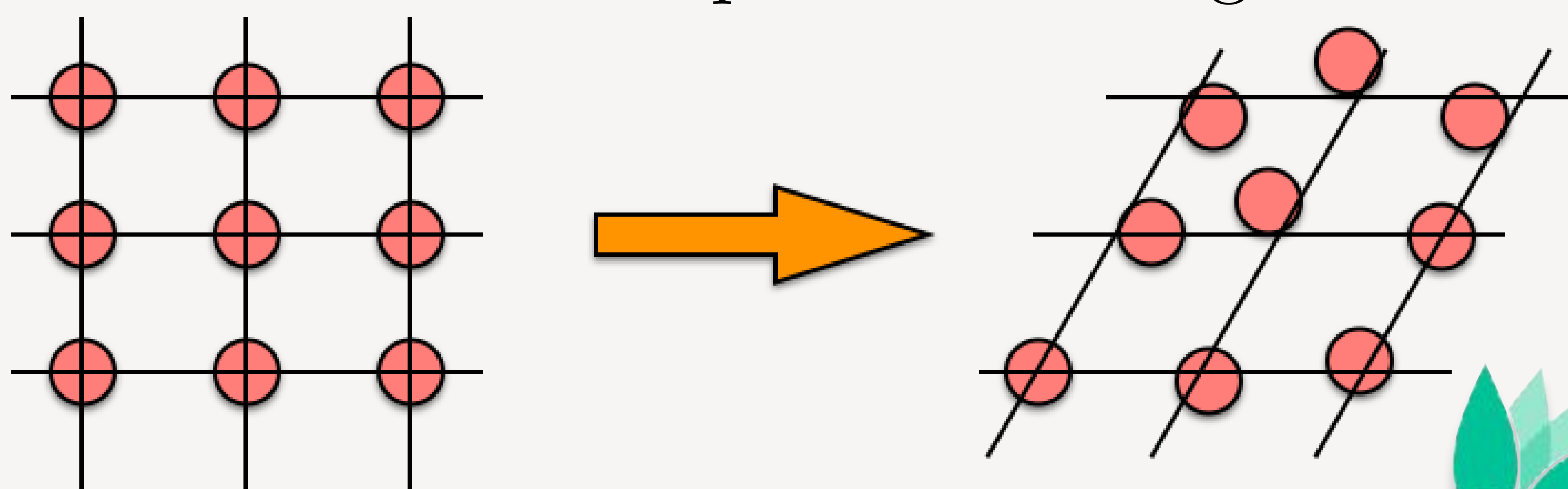
AFFINE AND NON-AFFINE

$$\{\mathbf{R}_i\} \to \{\mathbf{r}_i\} \;:\; (\mathbf{r}_i - \mathbf{r}_j) = \mathcal{D}(\mathbf{R}_i - \mathbf{R}_j)$$

Matrix $\mathcal{D}$ may be scalings, shear or rotations.



Displacements which cannot be represented using $\mathcal{D}$ are non-affine



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3 SOURCES OF NON-AFFINE DISPLACEMENTS

- Thermal fluctuations (Ganguly et al. , PRE 2013)
- Elastic heterogeneities (Di Donna and Lubensky, PRE 2005 and many others)
- Rearrangements (Nath et al. PNAS 2018)

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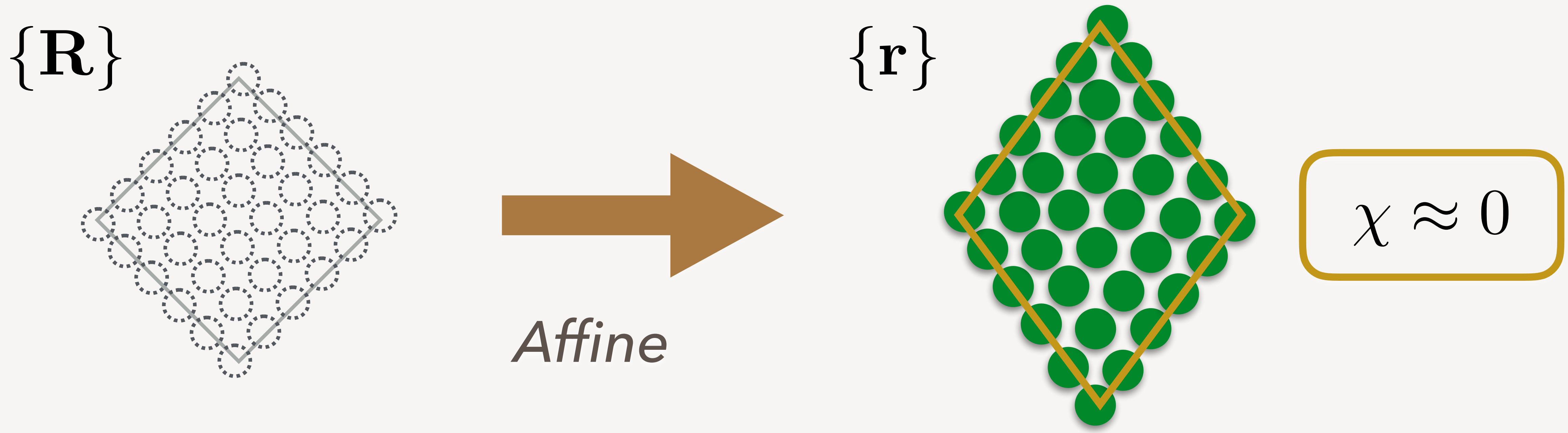
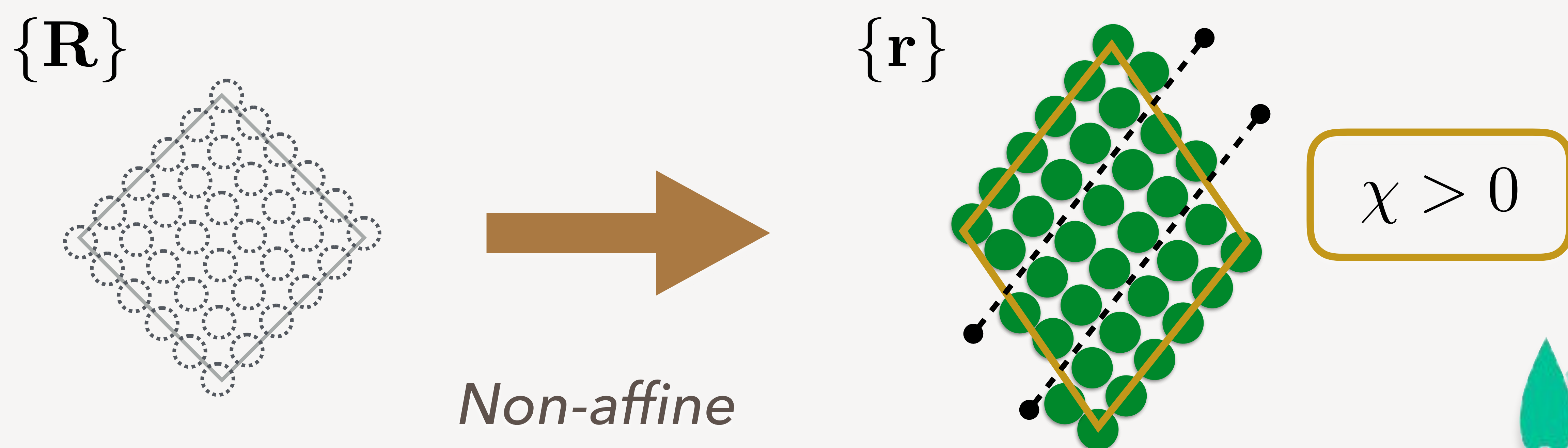
SPECIFICALLY

$$\boxed{\exists \quad \chi_\Omega(\{\mathbf{R},\mathbf{r}\}) \quad \forall \quad \{\mathbf{R}\},\{\mathbf{r}\}}$$

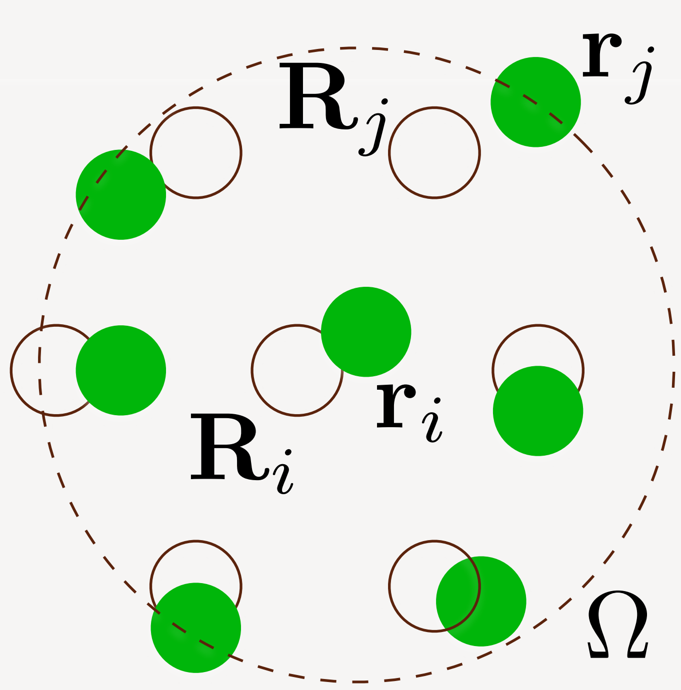


rearrangements cause non-affine-ness, measured by χ



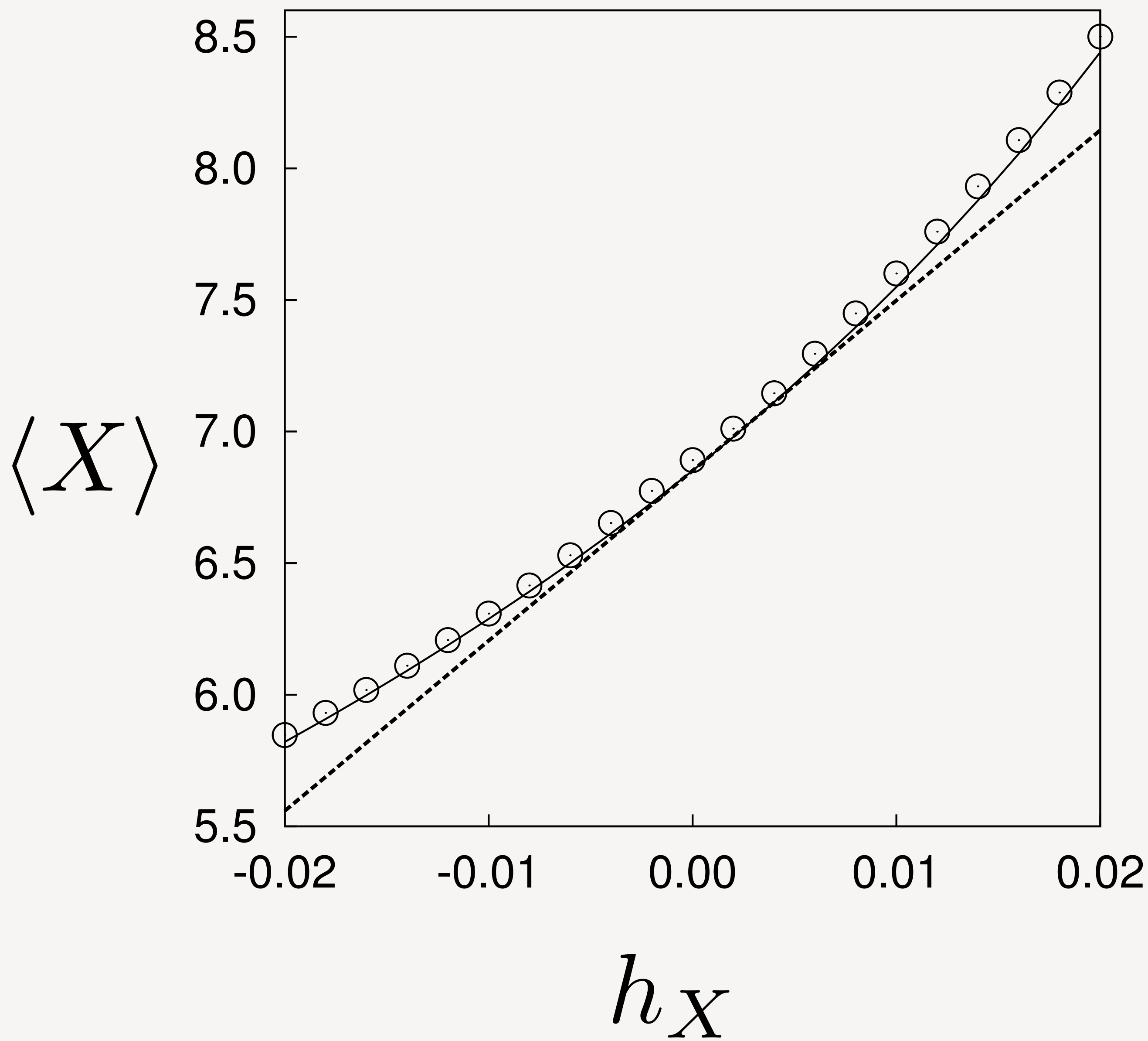
NON AFFINE DISPLACEMENTS

- Choose coarse graining volume Ω around a particle i.



BIASING NON-AFFINITY

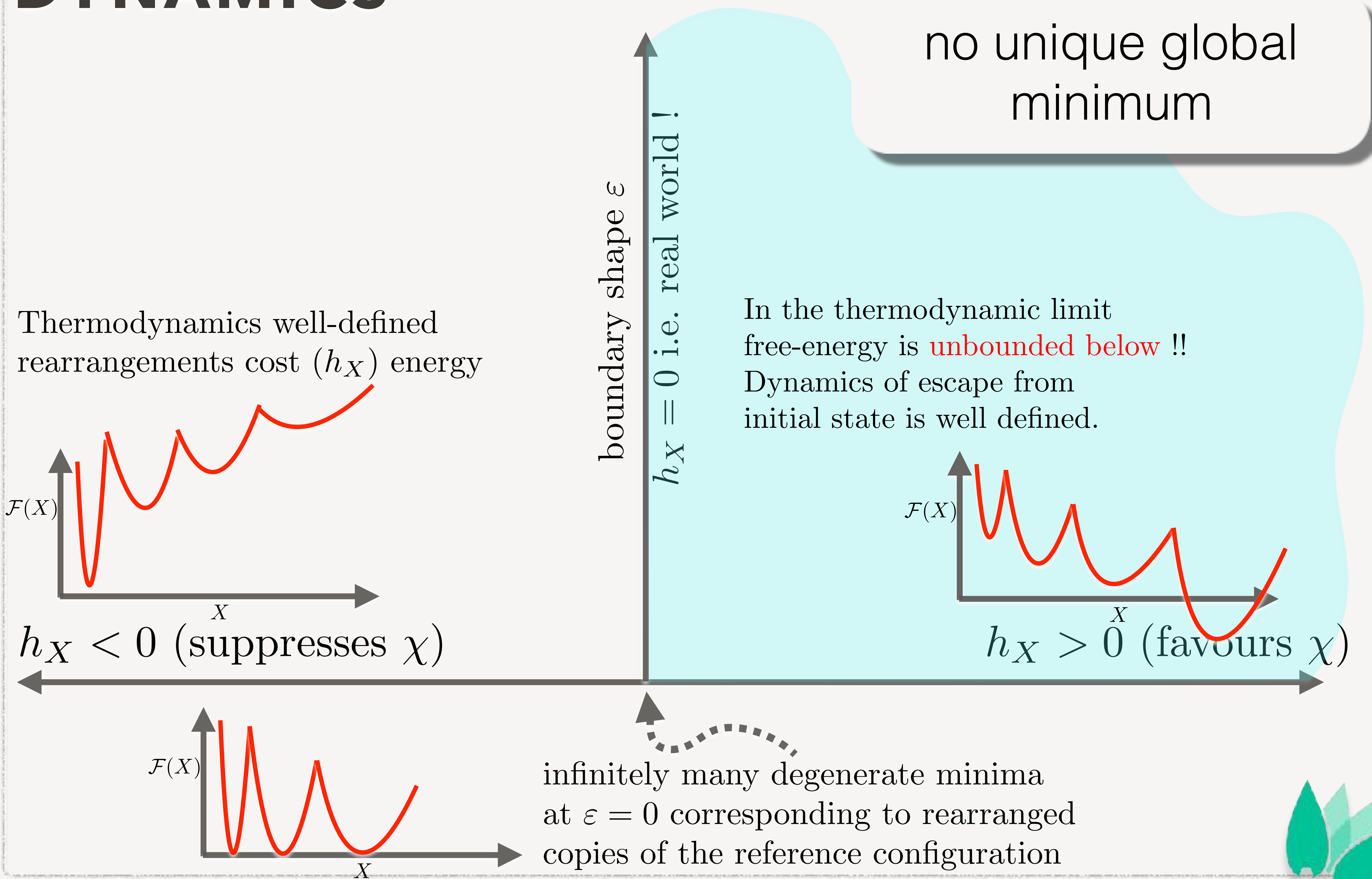
SMALL FIELDS: FLUCTUATION RESPONSE

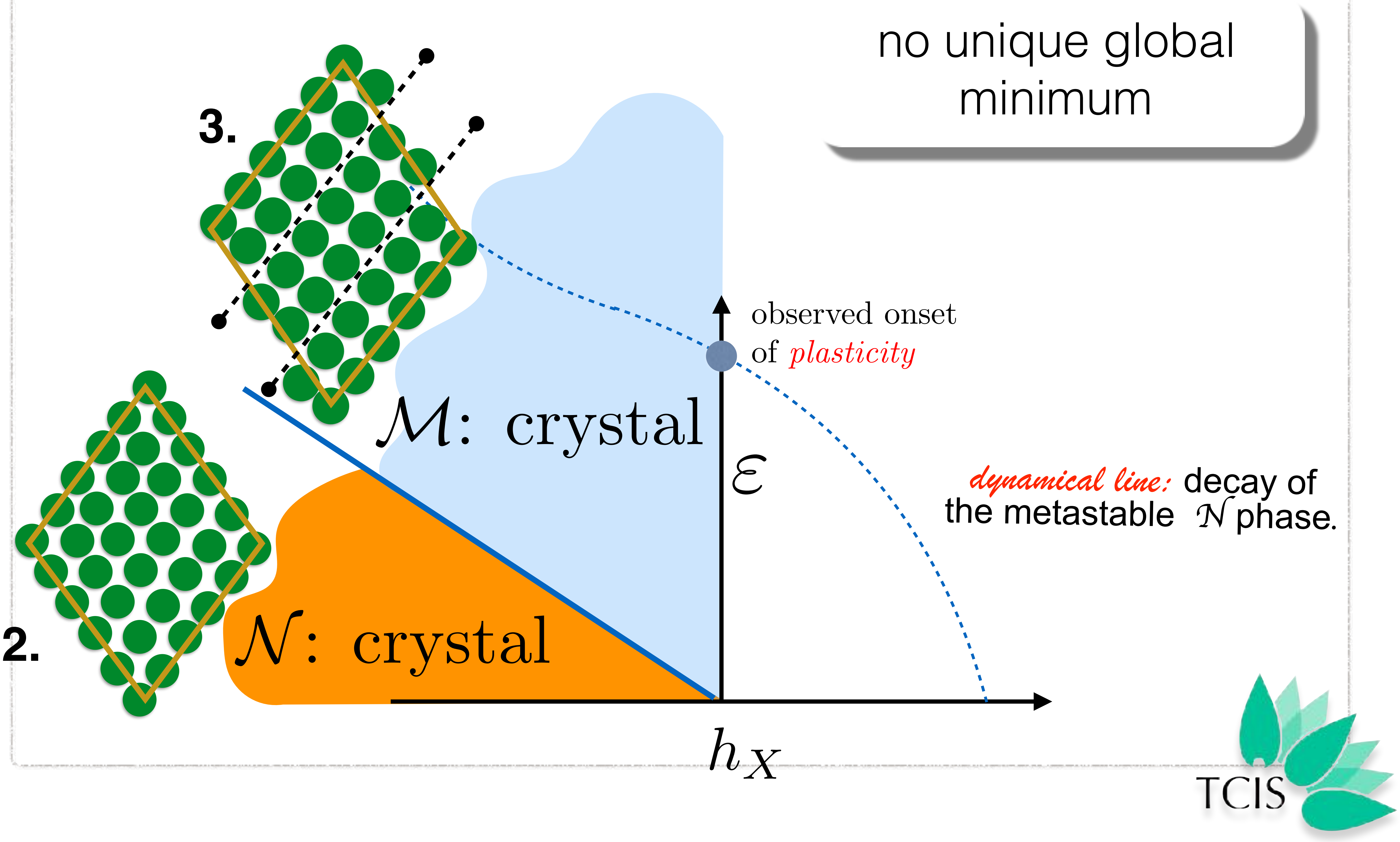


$X(h_X) = X(0) + \langle \Delta\chi^2 \rangle \sum_{\mathbf{R}} C_\chi(\mathbf{R}, 0)$ where $C_\chi(\mathbf{R}, 0)$ is the equal time, spatial correlation of χ.

S. Ganguly et al. Soft Matter, ***11****, 4517 (2015)* TCIS

LARGE FIELDS: GLOBAL THERMO-DYNAMICS




no unique global minimum
3.
2.
$\mathcal{M}$: crystal
$\mathcal{N}$: crystal
observed onset of *plasticity*
$\mathcal{E}$
h_X
dynamical line: decay of the metastable $\mathcal{N}$ phase.
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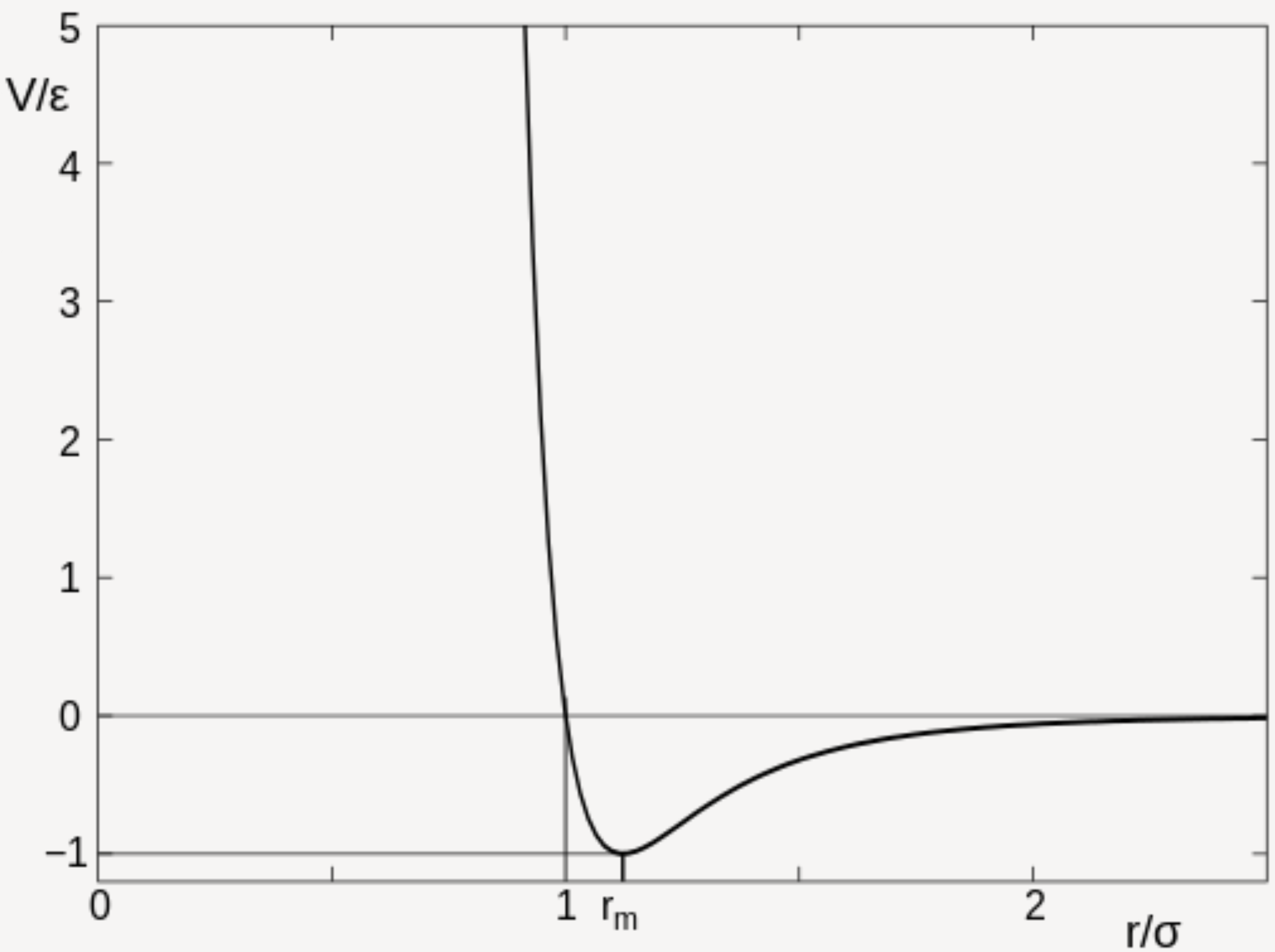
TWO DIMENSIONAL IDEAL LENNARD-JONES CRYSTAL

$$\boxed{V(r_{ij}) = 4\epsilon\left[r_{ij}^{-12} - r_{ij}^{-6}\right]}$$

- no pre-existing defects
- periodic boundary conditions
- constant NVT
- uniform (pure shear) by deforming the box.



Equilibrium $\rightarrow$ sequential umbrella sampling Monte Carlo

Dynamics $\rightarrow$ molecular dynamics simulations

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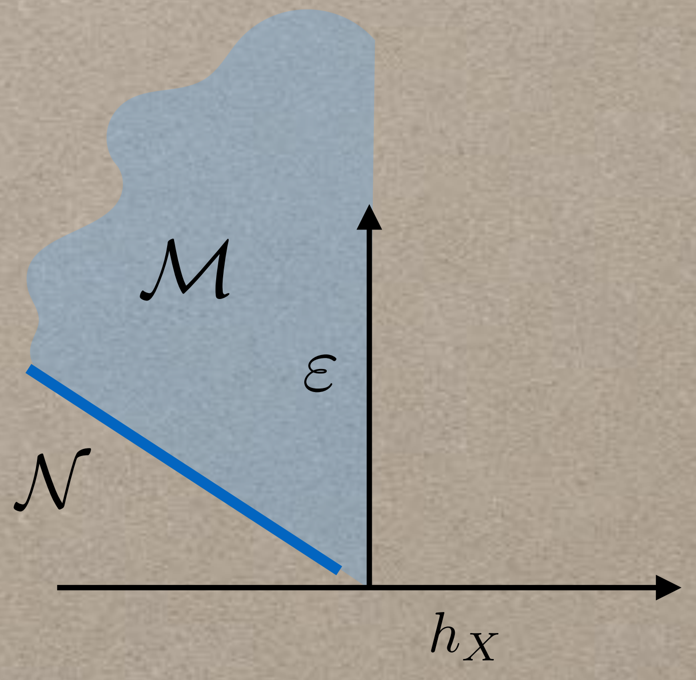
THE EQUILIBRIUM TRANSITION:
"X" as the order parameter



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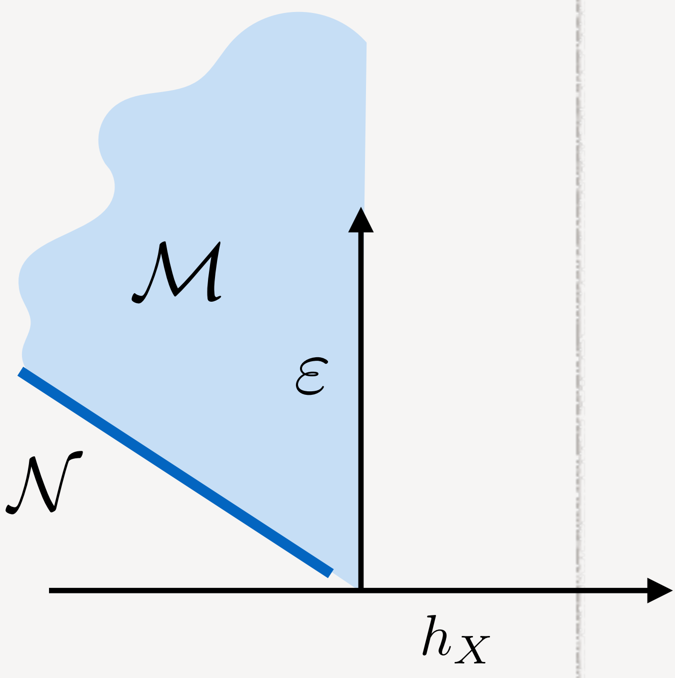
ENERGY BALANCE AND T=0 PHASE BOUNDARY



PHASE DIAGRAM AT T > 0

- N particles with Lennard Jones interactions in 2d plus non-affine field.
- constant $N, V(\text{shape}), T$, ensemble.
- cut-off at 2.5 times particle diameter, truncated and shifted, $T^* = 0.8, \rho = 2/\sqrt{3}$.
- Large energy barriers between $\mathcal{N}$ and $\mathcal{M}$ crystals.
- Sequential umbrella sampling Monte Carlo (SUS-MC) technique needed.
- accurate calculation of $P(X)$ at the transition.
- transition point obtained by histogram reweighting.

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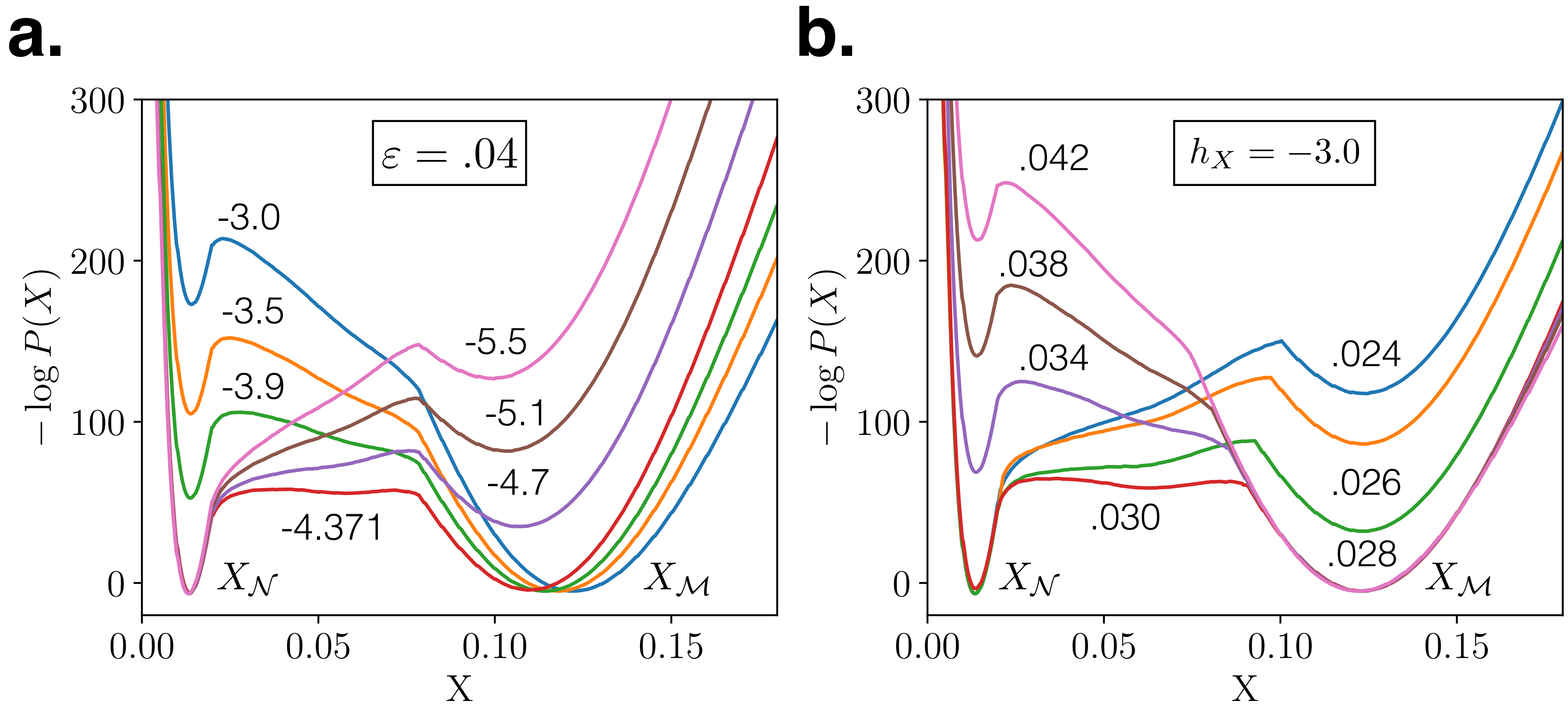
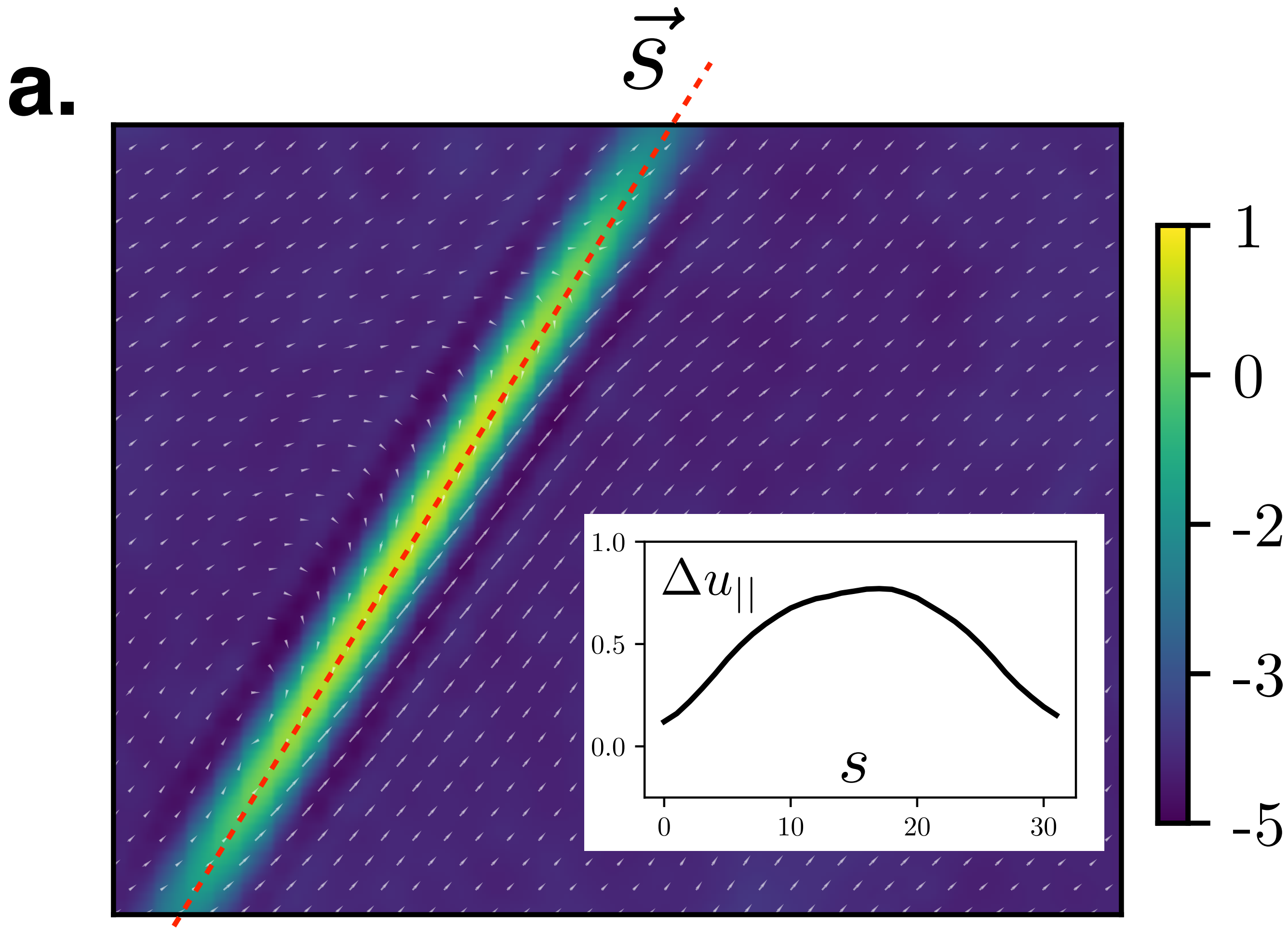
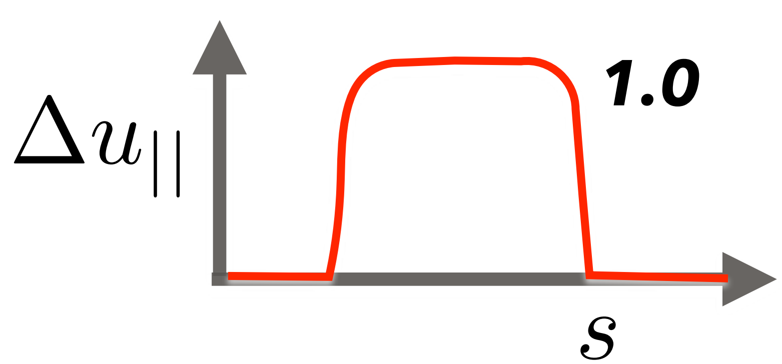
First order transition

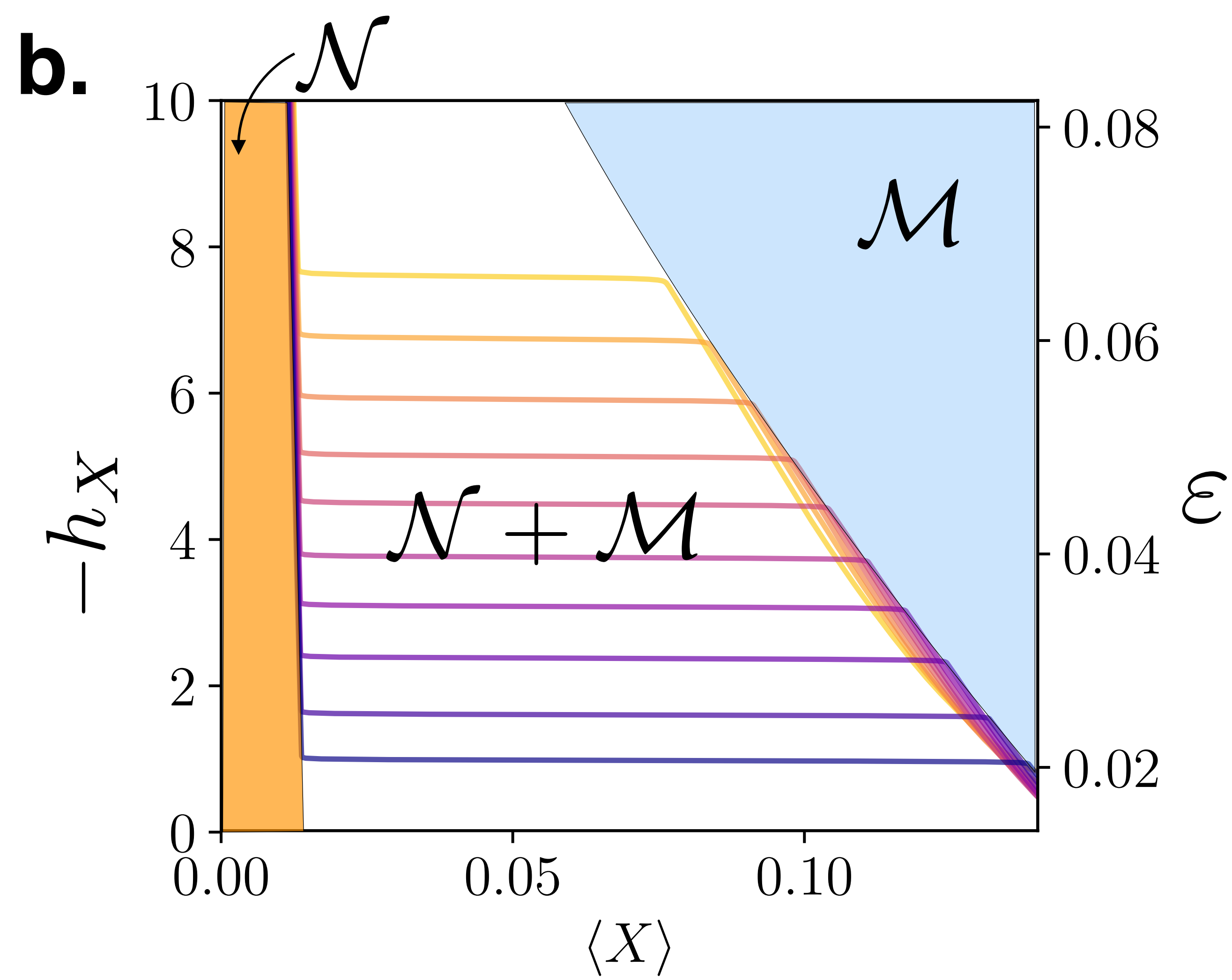


Slip bands, equation of state and phase diagram

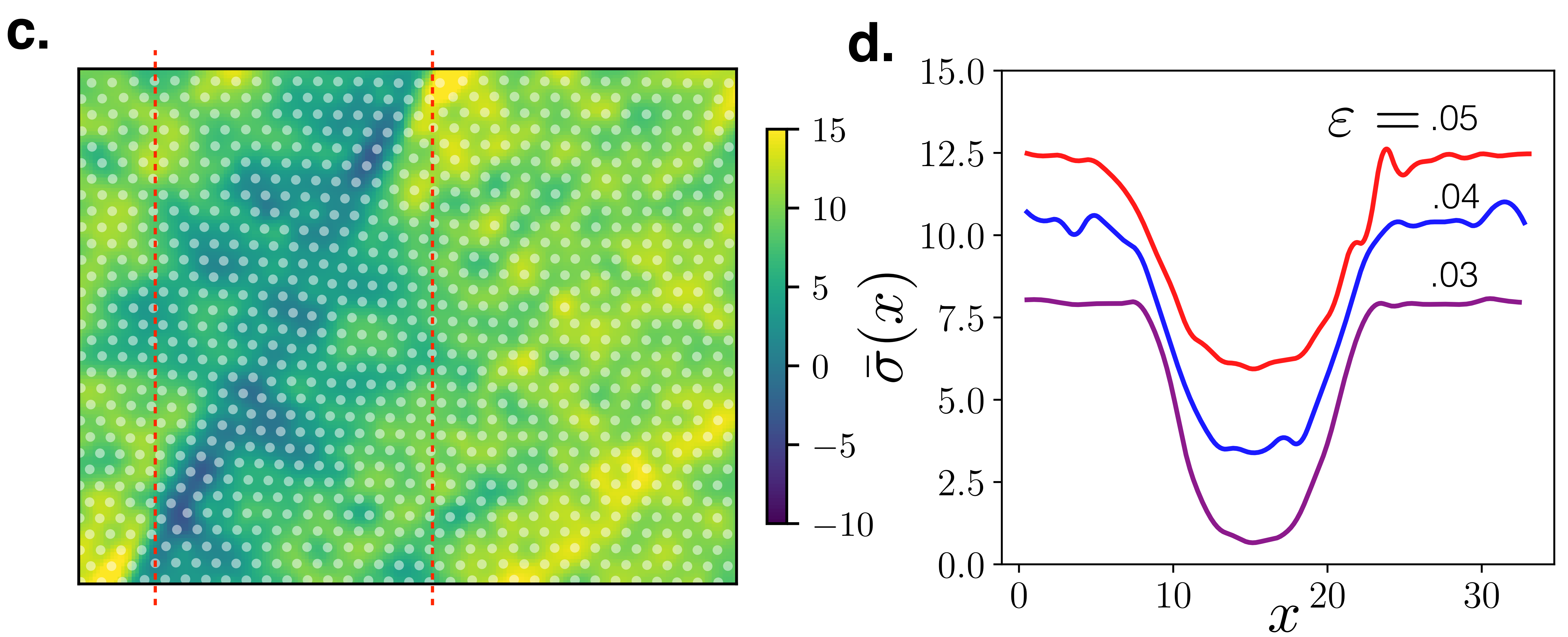


slip bands: *proto-* dislocation dipoles

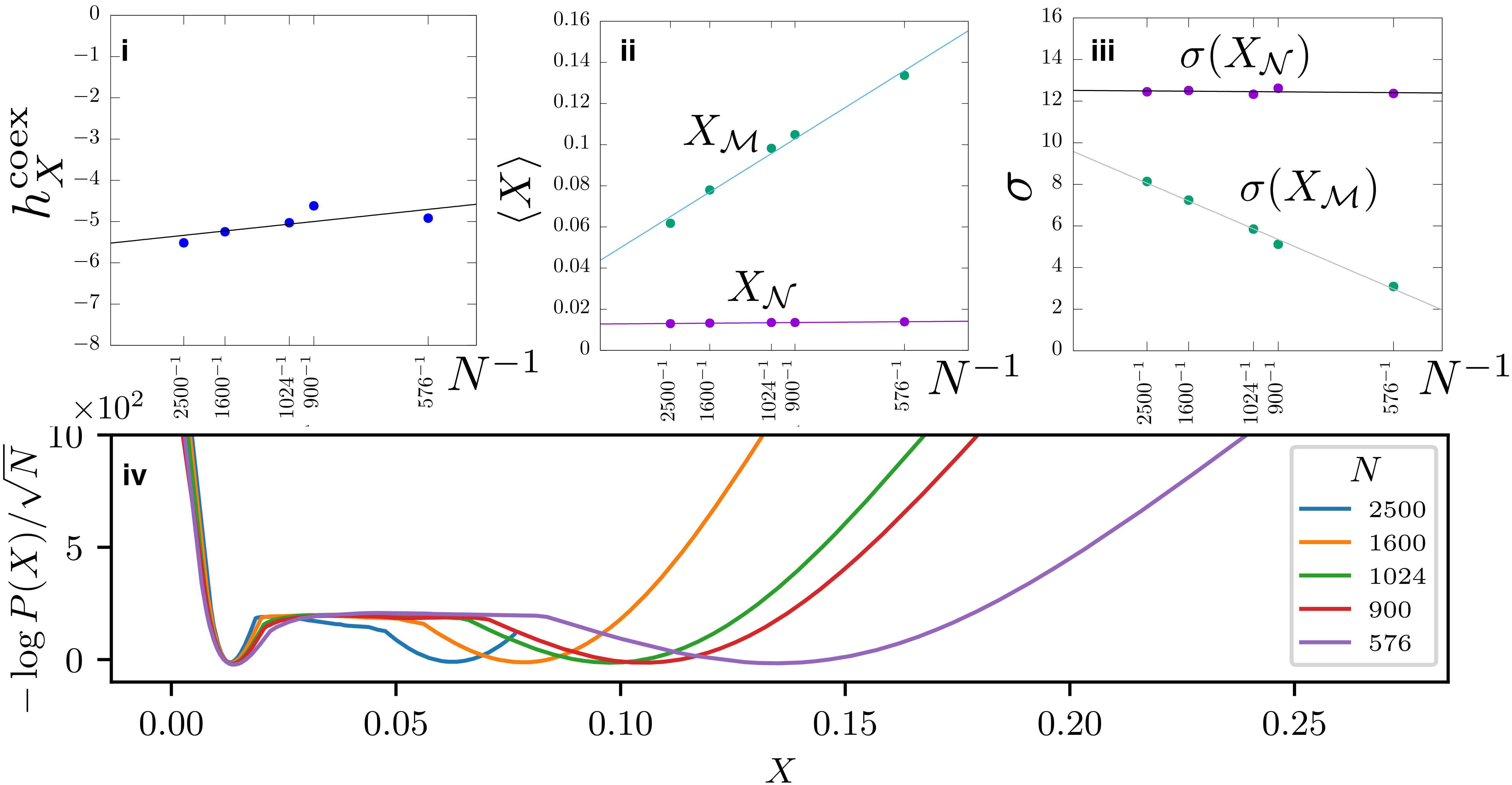




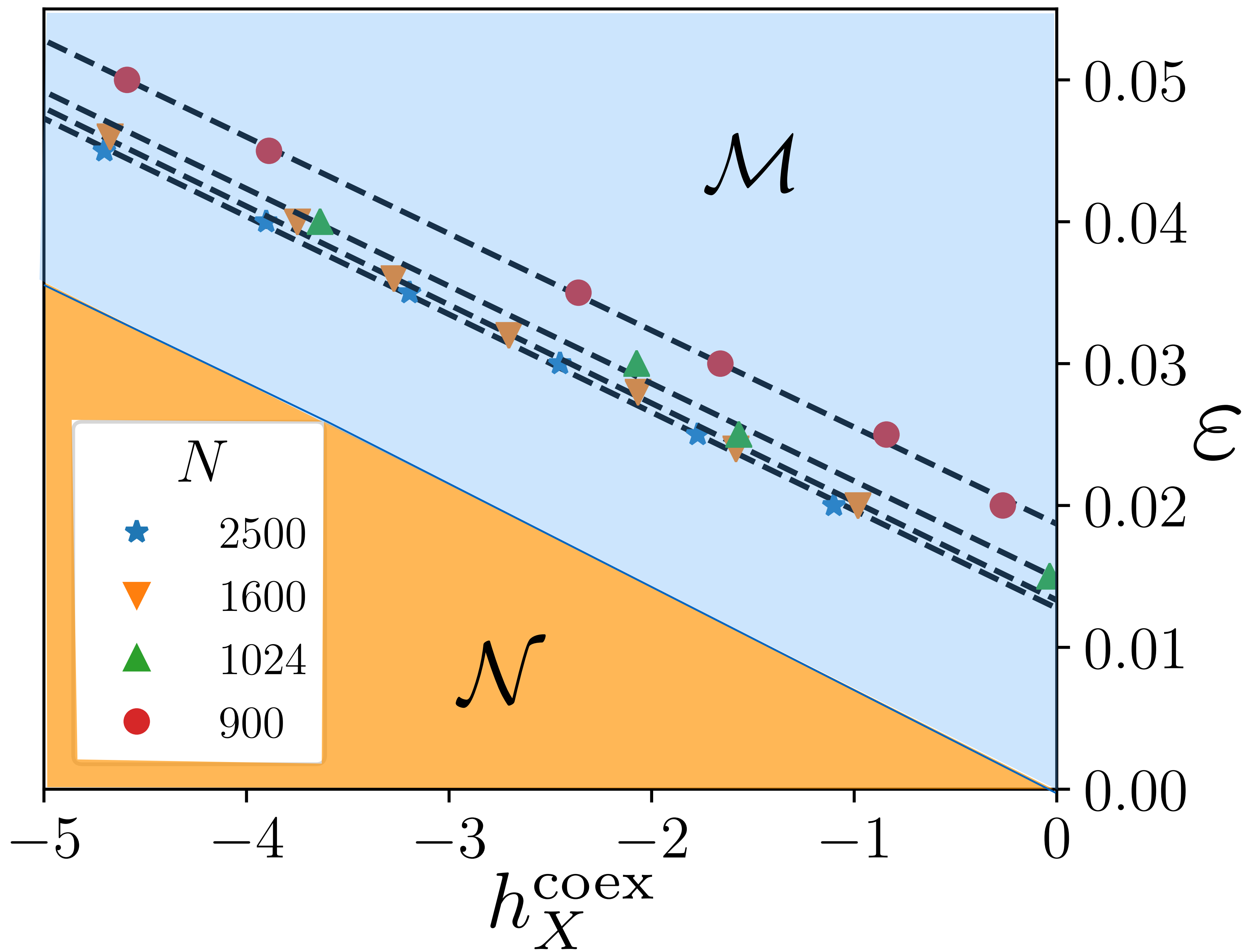
Stress interface



Finite size scaling



The phase diagram



SUMMARY

- First order phase transition between two equilibrium phases.
- Stable rigid crystal coexists with a new kind of crystal which responds to shape changes by producing slip bands and eliminating stress.
- Dislocations decorate stress interfaces - large stress gradients.
- Phase boundary extends to the origin, well defined in the limit, $h_X \to 0^-$
- The rigid crystal is metastable for all values of stress for $h_X = 0$.

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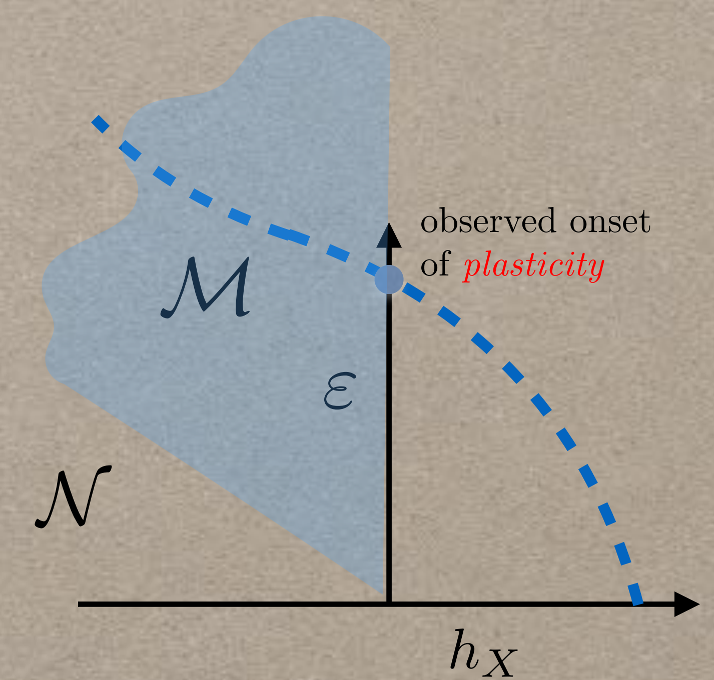
THE *DYNAMICS* AT FINITE STRAIN RATE:
"X" as a reaction coordinate



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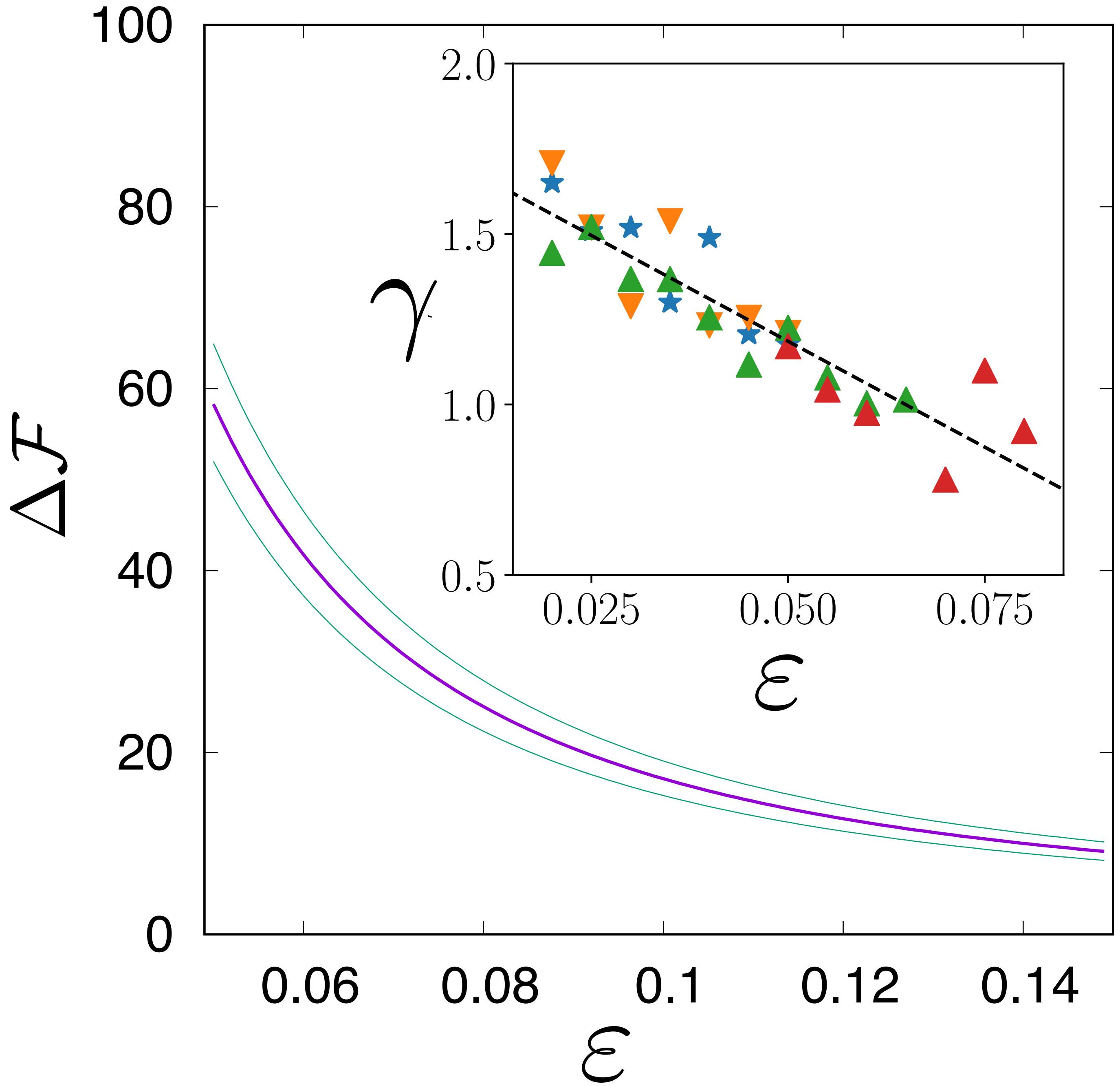
NUCLEATION BARRIERS AT h_x=0



$$\mathcal{F} = -\pi R^2 \Delta_b + 2\pi R\gamma$$

$$\Delta_b = \frac{1}{2}\sigma\varepsilon$$

γ from finite size scaling of SUS

$$\boxed{\Delta\mathcal{F} = \frac{\pi\gamma^2}{\Delta_b}}$$

Critical barrier height

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MD SIMULATIONS OF LJ SOLID

- $N = 128 \times 128 = 16384$ particles
- $a = 1.0$, $0.2 < T < 1.2$
- MD time step $\delta t = 0.001$, $= .0001$ near yielding.
- Berendsen thermostat
- equilibration for $t = 1500$
- strain rate $\dot{\varepsilon} = 3.33 \times 10^{-5}$ till yielding
- results averaged over 4 independent runs.
- fast GPU based in-house parallel code - checked against LAMMPS wherever possible.

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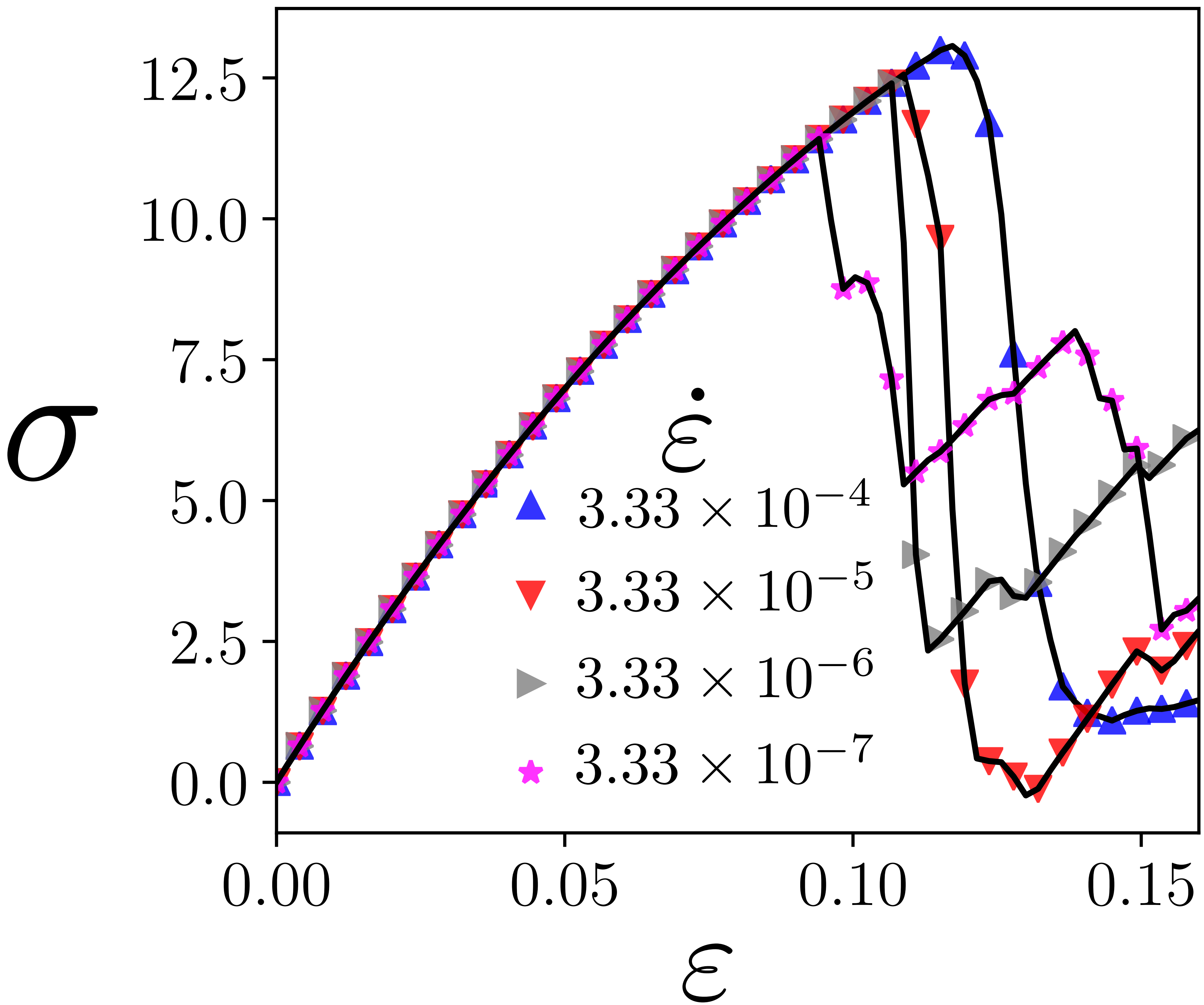

σ
12.5
10.0
7.5
5.0
2.5
0.0
0.00
0.05
0.10
0.15
ε
$\dot{\varepsilon}$
3.33×10^{-4}
3.33×10^{-5}
3.33×10^{-6}
3.33×10^{-7}

SELF CONSISTENT CNT

Strain ramped up in time $\rightarrow$ barrier $\Delta\mathcal{F}(t)$ is *time-dependent.*

$\therefore$ demand self consistency $\quad \tau_{FP} = \tau_0 \exp\left[\Delta\mathcal{F}(\tau_{FP})\right]$

multiply by $\dot{\varepsilon}$ and use, $\quad \dot{\varepsilon}\ \tau_{FP} = \varepsilon^*$

take logarithm $\quad \Delta\mathcal{F}(\varepsilon^*) = \log(\varepsilon^*) - \log(\dot{\varepsilon}\tau_0)$

Solved taking $\bar{\dot{\varepsilon}} = \dot{\varepsilon}\tau_0$ as a parameter.

Can use to obtain τ_0 from MD.

For CNT to be valid τ_0 must be constant.

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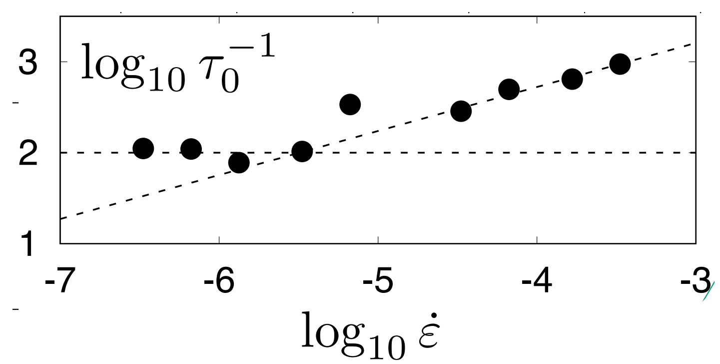
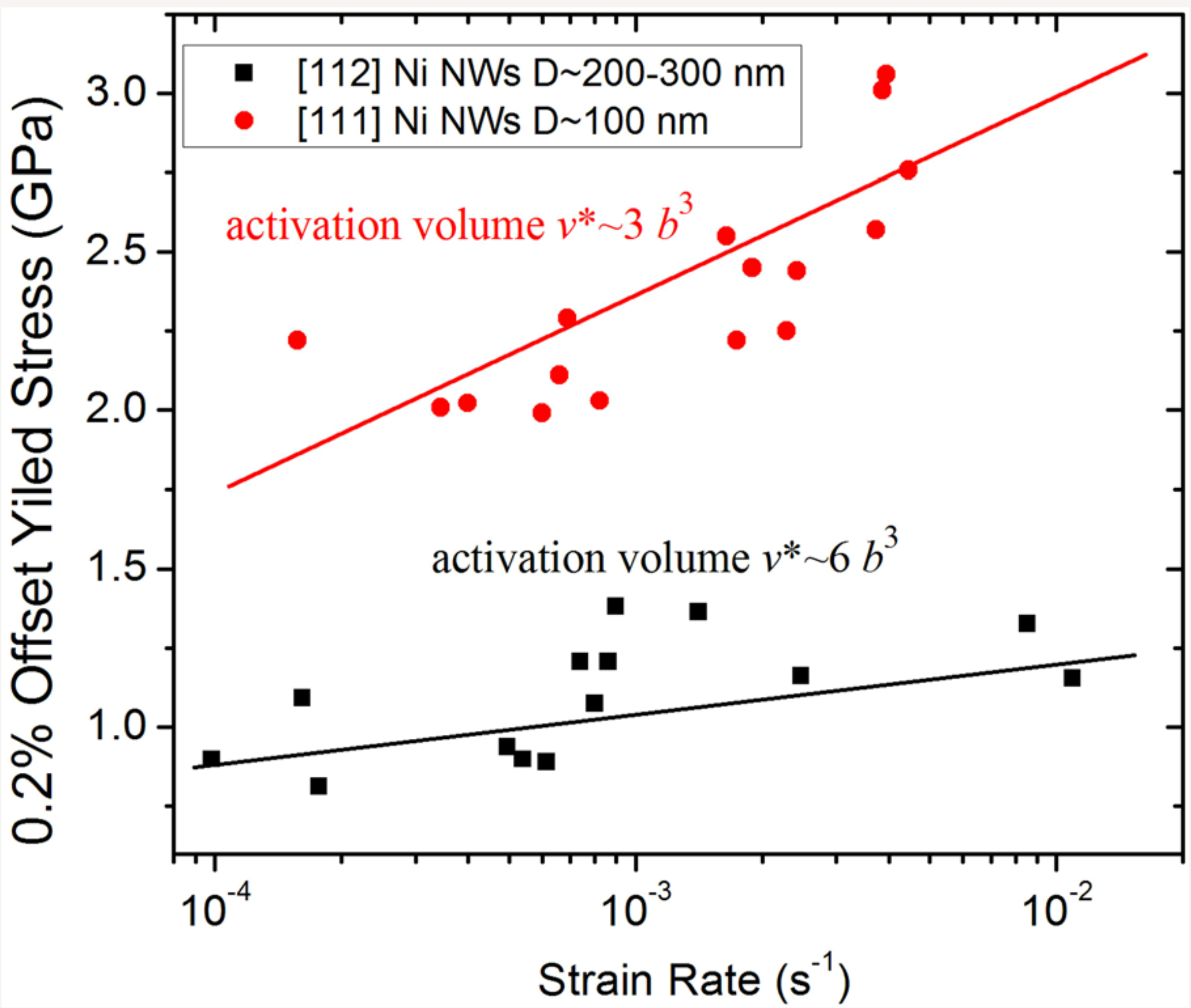
No “adjustable” parameters !!



Can predict $\varepsilon^*(\dot{\varepsilon})$ over the entire range of strain rates. Can determine range of validity of the nucleation picture. Such low strain rates are inaccessible in MD

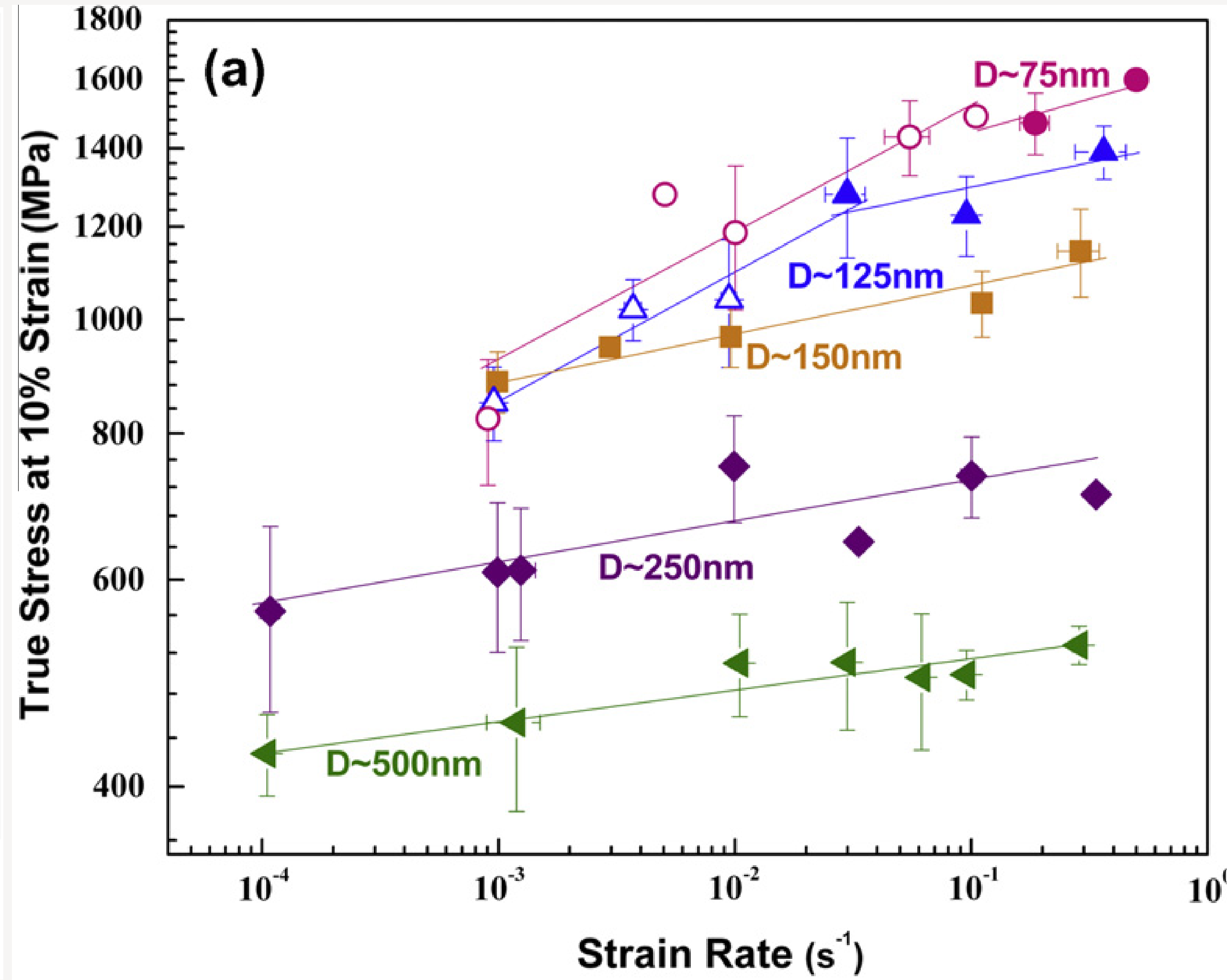
STRAIN RATE SENSITIVITY

Ni nano-wires



Peng et al. Appl. Phys. Lett. **102**, 083102 (2013)

Cu nano-pillars



Jennings et al. Acta Mat. **59**, *5627* (2011)

$$\cancel{\sigma = \sigma_0 \dot{\varepsilon}^m}$$

$$\boxed{\sigma = f(\log \dot{\varepsilon}); \ \lim_{x \to -\infty} f(x) = 0}$$

EXPLICIT "TAKE AWAYS"

- There exists a *hidden* first order transition between a rigid and a stress free crystal. All solids flow because a rigid solid is *always* in a metastable phase, which decays over time depending on the amount of deformation.

- Both equilibrium and non equilibrium aspects of this transition may be understood using a *new collective variable* X to distinguish affine and non-affine displacements.

- *Quantitative* prediction of rate dependent initiation of plasticity for the first time. Properties of dislocations *not needed* to discuss *onset of* plasticity of ideal crystals. Dislocations appear *only at coexistence* and only at the *stress interface*.

- New "picture" for deformation. Unifying *plasticity* with *first-order phase transitions*. To understand plasticity, concentrate on the *equilibrium transition*.

- May serve as a language for *plasticity* in solids where dislocations cannot be defined (*glasses*?).

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FROM CRYSTAL TO GLASS:
EFFECT OF A SINGLE FROZEN-IN DISLOCATION PAIR

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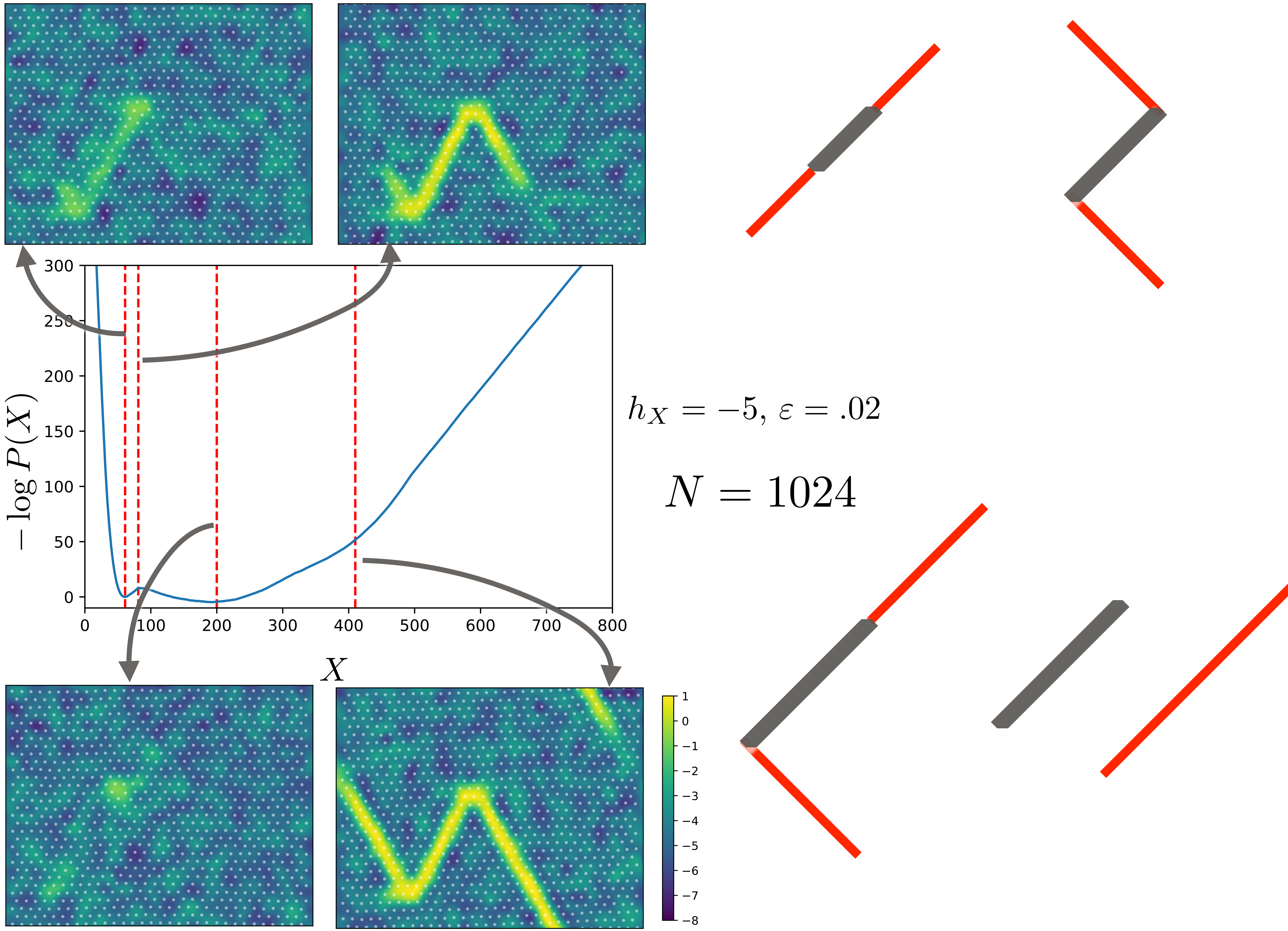

$-\log P(X)$
X
$h_X = -5,\ \varepsilon = .02$
$N = 1024$

SINGLE "FROZEN-IN" DISLOCATION DIPOLE

- Change in equilibrium phase boundary: M phase more stable.
- Barrier height becomes 1/5th: yield threshold decreases
- Kamer's regimes appears at much lower strain rates and spinodal regime becomes more dominant.
- Appearance of extra minima.
- Can already see what is expected for a glass!

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WHAT IS GOING ON?

A superconductor analogy ?

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- Superconductivity is associated with “gauge-symmetry breaking”.
- London equation $\mathbf{j} = -(n_s e^2/m)\mathbf{A}$ holds only in the Coulomb gauge, namely $\nabla \cdot \mathbf{A} = 0$.
- This leads to the Meissner effect i.e. elimination of flux.
- Gauge fixing happens naturally.
- Our case is analogous.
- Choosing reference lattice and h_X “fixes” a certain indexing. Local permutation symmetry is broken.
- Artificial gauge fixing $\rightarrow$ stress Meissner effect?
- In the real world only *kinetic* effects of this phase transition is felt.

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On the existence of thermodynamically stable rigid solids

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nanoscale views

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Sunday, June 24, 2018

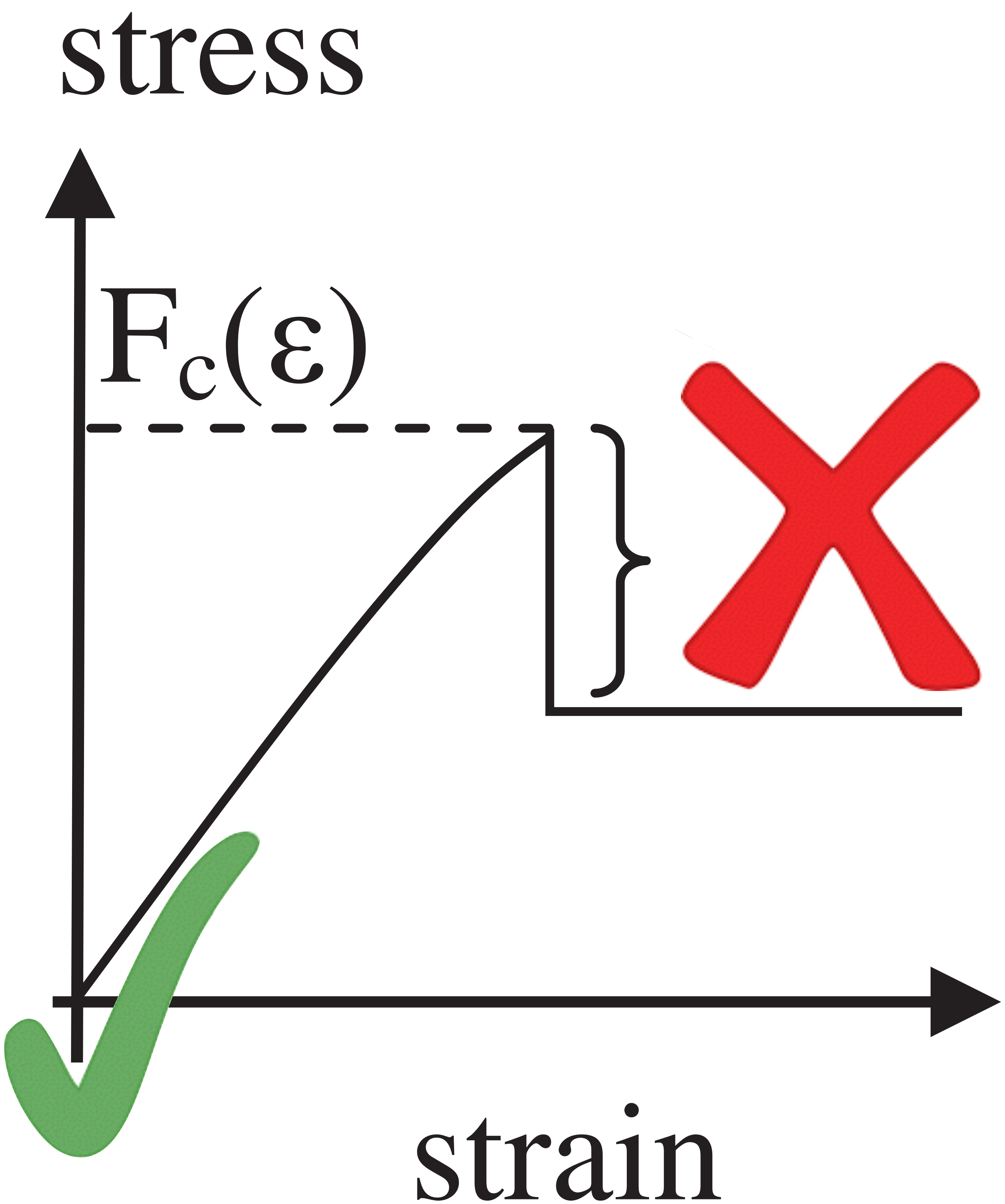
There is no such thing as a rigid solid.

How's *that* for a provocative, click-bait headline?

Books

http://nanoscale.blogspot.com/2018/06/there-is-no-such-thing-as-rigid-solid.html

TCIS


stress
Fc(ε)
strain

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