Deformation of crystals: Connections with statistical physics

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Table of Contents

Table of Contents

Crystals remember their shape. Broken translational order.

Memory in other non-equilibrium systems

Equilibrium erases the past. Non-equilibrium analogues?

Criticality and loss of memory

Are crystals scale invariant?

What kind of critical point? Self-organized?

What kind of critical point? Plain-old criticality?

Warning: Materials may be less universal. . .

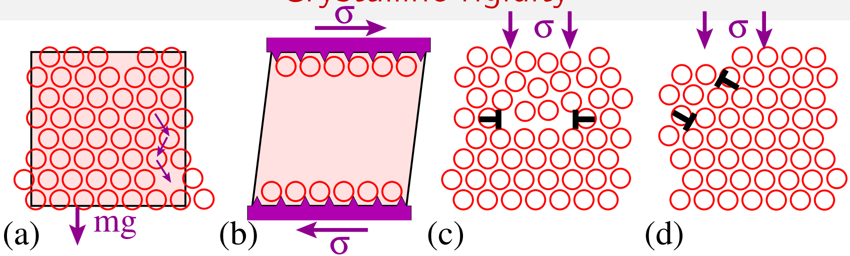
Bent spoon and yield stress: memory of shape

Metal spoon:

- Springs back (Hooke's law), soft ice-cream
- Bends (plastic deformation), too hard
- Many crystalline grains, regular grids of atoms
- Atomic planes must slide, rearrange: *dislocations*

The dynamics, interactions, and entanglement of these dislocation lines form the microscopic underpinnings of crystal plasticity.

Crystalline rigidity



Crystals:

(a) Flow like liquids under gravity[1]
(b) Rigid to shears σ that couple to broken translational symmetry
(c) Form dislocations when sheared more than half a lattice constant
(d) Dislocation *glide* at low temperatures

The nucleation rate of dislocation loops goes to zero faster than linearly as the compression goes to zero; there is no linear viscous flow response to forces that couple to the lattice. Crystals remember their shape.

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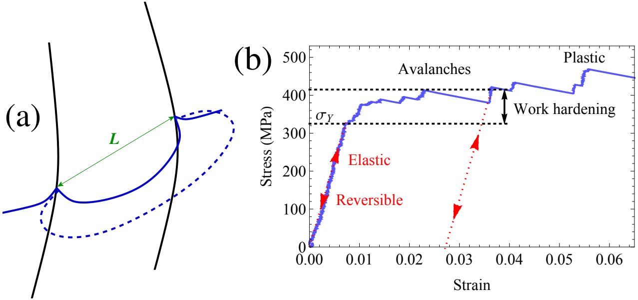
[1] via vacancy diffusion, above the surface roughening transition

Work hardening: memory of stress



(a) Dislocations tangle and pin. Stress σ causes ballooning, triggering avalanches.
(b) Micropillar deformation, Hooke's law until σ_Y, then avalanches and plasticity.[2]

New dislocations raise the yield stress σ_Y, leading to *work hardening* – a stress memory.

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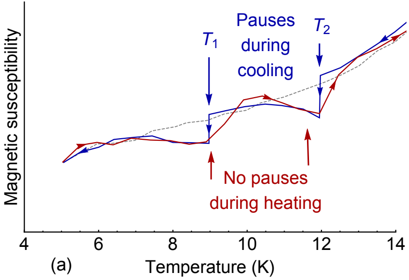
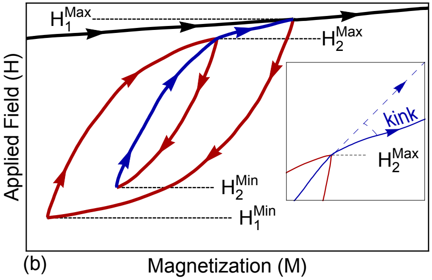
[2] From Xiaoyue Ni, Haolu Zhang, Danilo Liarte, Louis W. McFaul, Karin A. Dahmen, JPS, Julia R. Greer, 'Precursor dislocation avalanches in small crystals: The irreversibility transition'.

Table of Contents

Magnetic memory of heating and beating





(a) Spin glasses are frustrated. Annealing on cooling T_1, T_2 leaves fewer active modes upon heating.[3]

(b) Magnets often have *return-point memory* – they return to precisely the same microstates after subloops, leading to kinks in $M(H)$.[4]

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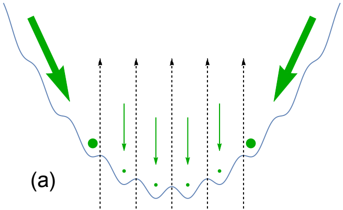
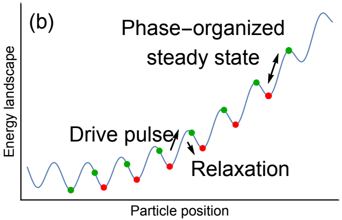
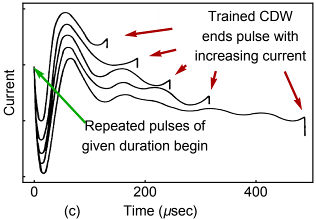
[3] Jonason K, Vincent E, Hammann J, Bouchaud J, Nordblad P, *PRL* **81**, 3243 (1998).

[4] JPS, Dahmen K, Kartha S, Krumhansl JA, Roberts BW, Shore JD, *PRL* **70**, 3347 (1993).

Phase organization: Memory and training







System history selects unusual metastable states.

(a) Nail, ball, periodic potential. Basin of extremal states much larger than typical. Hypercorners of hypercube selected.[5]

(b) Training by driving for fixed duration: green is endpoint; selects states at peak of energy.

(c) Charge-density wave materials, trained to different durations, always have increasing current at *end* of pulse.[6] [7]

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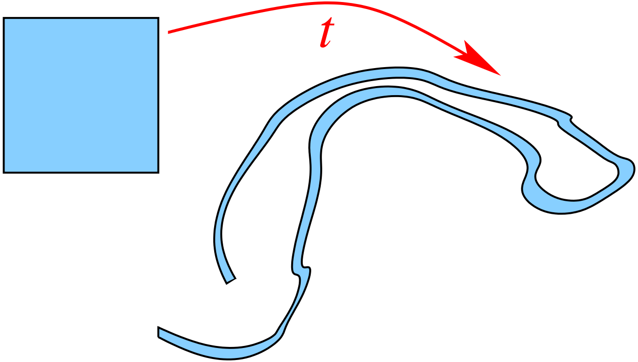
[5] Coppersmith S, *Phys. Lett. A* **125**, 473 (1987).

[6] Coppersmith S, Littlewood P, *PRB* **36**, 311 (1987)

[7] Tang C, Bak P, Coppersmith S, Littlewood P, *PRL* **58**, 1161 (1987).

Table of Contents

Equilibrium: erasing the past



Equilibrium systems are simple.

(1) Their dynamics is chaotic: erasing all information except for conserved quantities and broken symmetries.

(2) Energy-conserving Hamiltonian dynamics preserves volume in phase space (Liouville's theorem).

All states at fixed energy have the same probability per unit phase space volume.

Non-equilibrium thermodynamics? Forgetting the history

Fixed relative probabilities for metastable states (point configurations). (No phase organization, return-point memory, thermal history memory.)

- Edwards' theory of powders: equal weights, fixed density (compactivity)[8]
- Chakraborty and Edwards: powders at fixed density and external force (angoricity)[9][10]
- Effective temperature: weight by energy (effective temperature):
  - Glasses and amorphous metals (Langer, Bouchbinder, Manning, Cugliandolo, Kurchan, Ono, Barrat, Berthier)
  - Polymers (Xiao, Nguyen)
  - Dislocations (Langer)

Can a non-equilibrium system forget its history, and partition its state equally among a discrete family of configurations?

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[8] Edwards S, Oakeshott R. *Physica A Stat. Mech. Appl.* **157**, 1080 (1989).

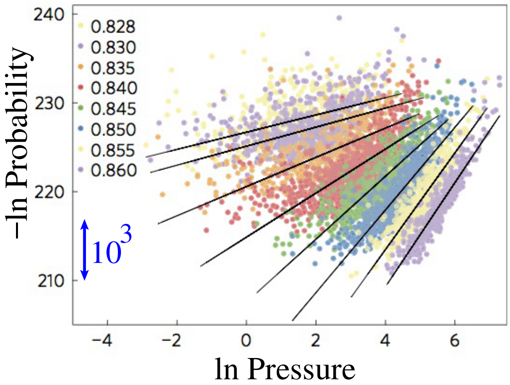
[9] Henkes S, Chakraborty B, *PRL* **95** 198002 (2005).

[10] Blumenfeld R, Edwards S., *J. Phys. Chem. B* **113** 3981 (2009).

Table of Contents

Grains forget only at jamming transition

- Daniels found compactivity violates zeroth law[11]
- Martiniani numerically checked the relative probability of all stable configurations (one history).[12]
- Fixed density, broad range of probabilities
- Fixed pressure also, narrower range.
- As pressure goes to zero (the jamming transition) distribution becomes narrower (range 10^3)



Scaling extrapolation suggests equal probabilities: entropy is maximized at jamming.

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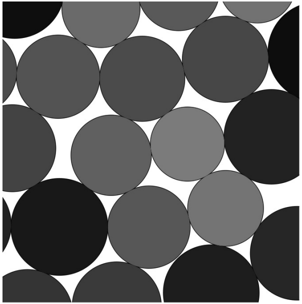
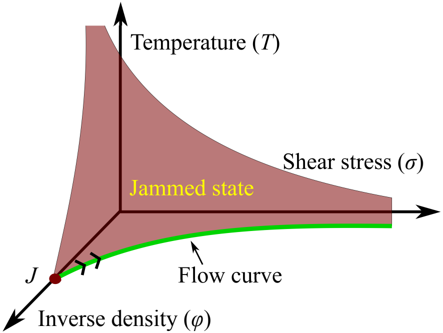
[11] Puckett JG and Daniels KE, *PRL* **99**, 038002 (2007).

[12] Martiniani S, Schrenk KJ, Ramola K, Chakraborty B, Frenkel D, *Nature Phys.* **13**, 848 (2017).

Jamming





Jamming describes the onset of rigidity of hard particles.[13]

- Jammed at low T, low shear σ, high density
- Jamming point J shows power laws, scaling collapses, and diverging lengths
- Scaling *ansatz* argues[14] the free energy
  $$F(\Delta\varphi, P, \sigma, T) = \Delta\varphi^2 \mathcal{F}_0(P/\Delta\varphi, \sigma/\Delta\varphi^{5/4}, T/\Delta\varphi^2).$$

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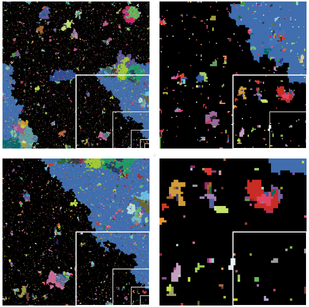
[13] Liu AJ, Nagel SR *Ann. Rev. Condens. Mat. Phys.* **1** 347 (2010)

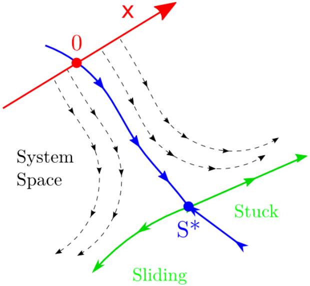
[14] Goodrich CP, Liu AJ, JPS, *PNAS* **113** 9745 (2016).

Memory loss at critical points

The renormalization group

- Flow in ‘system space’
- Space includes models and experiments
- Flow describes coarse-grained model at longer length scales.
- At critical point, *scale invariant*



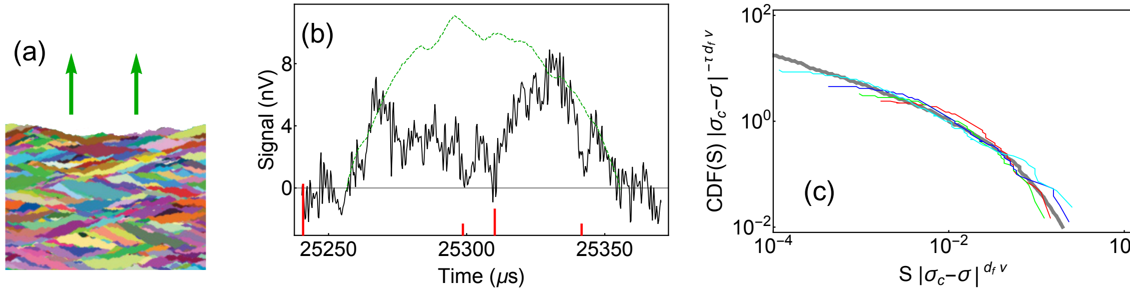


- Tuning a parameter through critical point O.
- Critical point flows to fixed point S^*, hence is self similar.
- All blue curve points flow to same S^*, universal.
- Near the critical point, power law scaling, universal exponents and scaling functions.

Universality implies that memory on long scales is embedded in a finite number of relevant parameters (plus corrections to scaling).

Table of Contents

Avalanches



Avalanches: scale invariant in space, time, and size

(a) Coffee invading a napkin[15]

(b) Avalanche fractal in time t, average shape universal parabola[16] (green)
$\langle V(t|T)\rangle \sim T^{1-d_f/z}\mathcal{V}(t/T)$

(c) Micropillar avalanches cut off, diverge at failure stress (theory: gray curve) [17]

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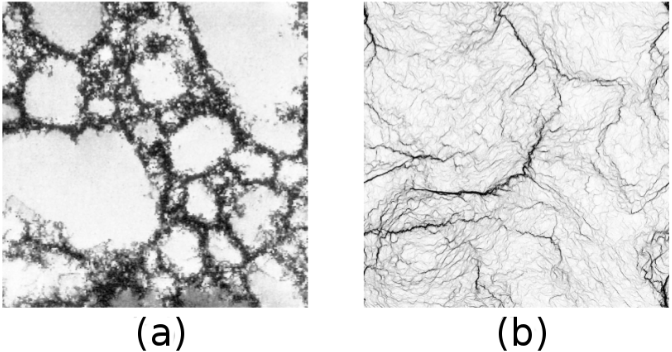
[15] Chen Y, Papanikolaou S, Sethna JP, Zapperi S, Durin G, *PRE* **84** 061103 (2011).

[16] Papanikolaou S, Bohn F, Sommer RL, Durin G, Zapperi S, JPS *Nat. Phys.* **7** 316, 2011.

[17] Friedman *et al.*, *PRL* **109**, 095507 (2012) [w/Greer, Dahmen].

Cell structures & scaling



(a) Dislocation *cell structures* display structure on many length scales.[18]

(b) Continuum model exhibits power laws and scaling, experimental features[19][20]

What kind of critical point?

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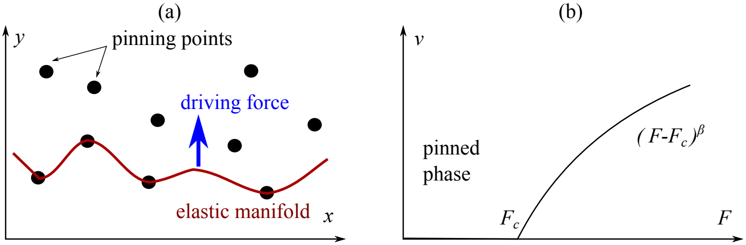
[18] Hähner P, Bay K, Zaiser M, *PRL* **81** 2470 (1998).

[19] Chen YS, Choi W, Papanikolaou S, Bierbaum M, JPS, *Int. J. Plast.* **46** 94 (2013).

[20] Chen YS, Choi W, Papanikolaou S, JPS *PRL* **105** 105501 (2010).

Table of Contents

Depinning and criticality



Depinning transitions[21]

(a) Jerky movement of surfaces pinned by disorder as they are dragged

- Planar cracks, superconducting vortices, raindrops on windshields, . . .
- Avalanches between metastable states

(b) Plain-old critical when external force fixed

- Self-organized critical when driven slowly (earthquakes)
- Dislocations thought self organized due to work hardening

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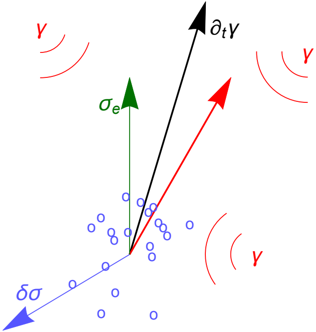
[21] Fisher DS, *Phys. Rep.* **301** 113 (1998).

Mesoscale plasticity[22]

$$\frac{1}{B}\partial_t\gamma(\mathbf{r}) = \sigma_{\text{ext}} + \sigma_{\text{int}}(\mathbf{r}) + \delta\sigma(\mathbf{r},\gamma)$$

$$\sigma_{\text{int}}(\mathbf{k}) = -\frac{G}{\pi(1-\nu)\gamma(\mathbf{k})}\frac{k_x^2k_y^2}{|\mathbf{k}|^4} \tag{1}$$



- Dislocation slip γ, external driving σ_{ext}, nonlocal interactions σ_{int}, dirt and entanglement $\delta\sigma(\mathbf{r},\gamma)$
- Dislocation stress can both increase and decrease from slip (not convex)
- Dislocations tangle even without dirt (generate own disorder, like glasses)

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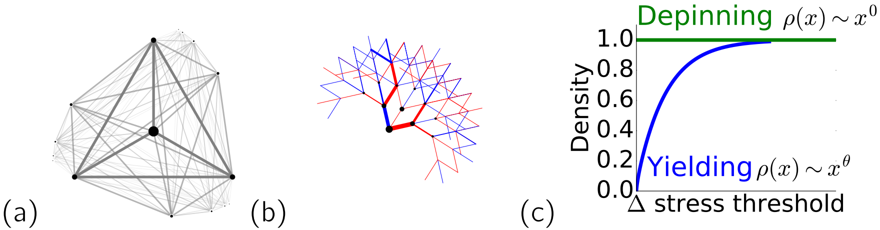
[22] Zaiser M, *Adv. Phys.* **55** 185 (2006).

Mean field theory & plasticity



Mean field theories describe systems in high dimensions or with long-range forces.

(a) Mean-field of all other sites: hypertetrahedron

(b) High dimensions: infinite branching tree (Bethe lattice).

- Avalanche creates an anisotropic strain, positive and negative stresses

(c) Ignore anisotropy: decreases give pseudogap,[23] $\tau \leq 3/2$

- Anisotropy may allow decreases to be ignored,[24] giving $\tau = 3/2$?
- Experiments and simulations give many different τs

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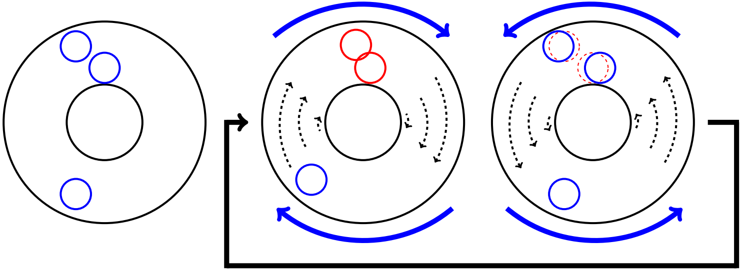
[23] Lin J, Wyart M, *PRX* **6**, 011005 (2016).

[24] Fisher DS, Dahmen KA, Ramanathan D, Ben-Zion Y, *PRL* **78** 4885 (1997).

Table of Contents

Hysteresis, reversibility, and irreversibility[25]



- Low Reynold's number reversible on oscillation
- Colloidal particles reverse unless they collide (avalanches)
- Small amplitudes *trainable*: few small collisions decay under cycling
- Like plasticity, new collisions when amplitude increases
- Large amplitudes *untrainable*: collisions never cease
- Critical amplitude: 'reversible-to-irreversible' (RIT) trainability transition
- Diverging training times and amplitudes.

Also in amorphous solids, granular systems, dislocations, superconducting vortices.

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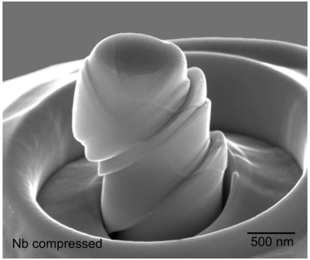
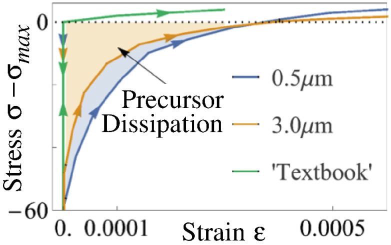
[25] Corté, Pine, Chaikin, Gollub, Paulsen, Keim, Nagel, Reichhardts, . . .

Nanopillar precursor avalanches





Micropillars squash via dislocation avalanches.[26]

- Textbooks: Hooke until yield stress $\sigma_Y = \sigma_{\max}$, previous maximum stress (self-organization)
- Micropillars: *precursor avalanches* upon reloading below $\sigma_{\max}$
- Precursors average into the stress-strain curves at right.
- Smaller pillar has larger precursors; vanish in macroscopic samples?

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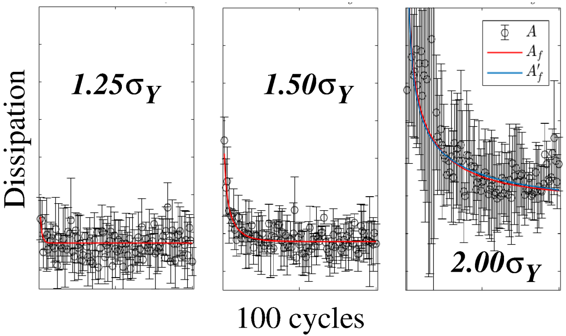
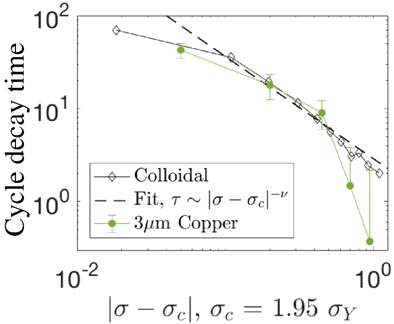
[26] Xiaoyue Ni, Haolu Zhang, Danilo Liarte, Louis W. McFaul, Karin A. Dahmen, JPS, Julia R. Greer, 'Precursor dislocation avalanches in small crystals: The irreversibility transition'.

Reversible-irreversible transition in micropillars[27]





- Failure stress σ_c
- $\sigma_{\max} < \sigma_c$ trainable; avalanches disappear with cycles
- $\sigma_{\max} > \sigma_c$ continues to squash forever
- Training cycle decay time, amplitudes diverge at σ_c
- Behavior compares well to colloidal system data

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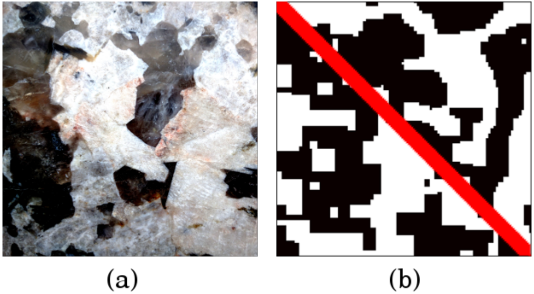
[27] Xiaoyue Ni, Haolu Zhang, Danilo Liarte, Louis W. McFaul, Karin A. Dahmen, JPS, Julia R. Greer, 'Precursor dislocation avalanches in small crystals: The irreversibility transition'.

Table of Contents

Non-universality



Bewildering variety of real materials. Hope for 'universal' scaling theory of plasticity?

(a) Polycrystalline granite: scaling theory of coarsening.
  - Salad dressing universal, but here facets.

(b) Facets in 3D Ising model, with\without nn bonds[28][29]
  - Anisotropic surface energies, mobilities 'relevant variables' for coarsening

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[28] Shore JD, Holzer M, JPS, *PRB* **46**, 11376 (1992).

[29] Rutenberg AD, Vollmayr-Lee BP, *PRL* **83**, 3772 (1999).