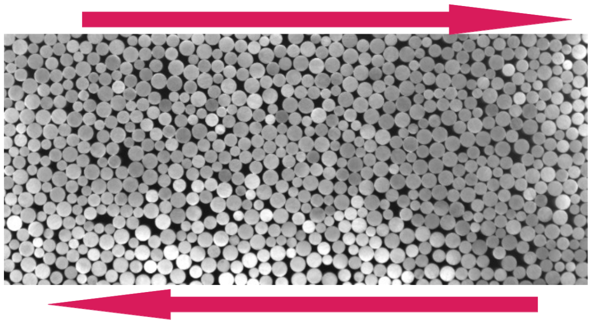
The fate of shear-oscillated amorphous solids

C. Liu, EE Ferrero, EA Jagla, K Martens, A Rosso, L Talon, J. Chem. Phys. 156, 104902 (2022)



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IDE-GDR workshop – Grenoble (France)
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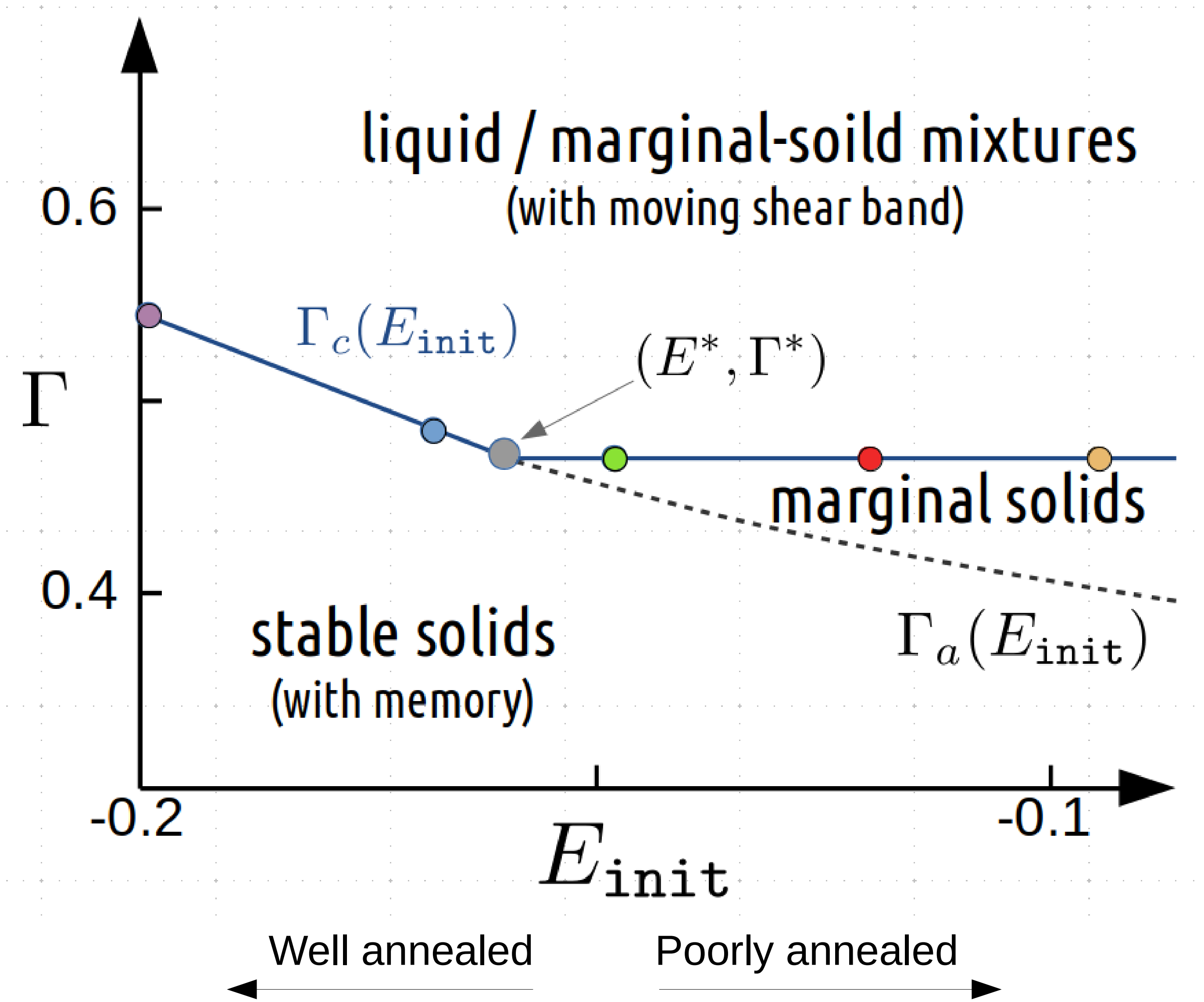
The fate of shear-oscillated amorphous solids

Steady-state is fully determined by the initial preparation and the oscillation amplitude



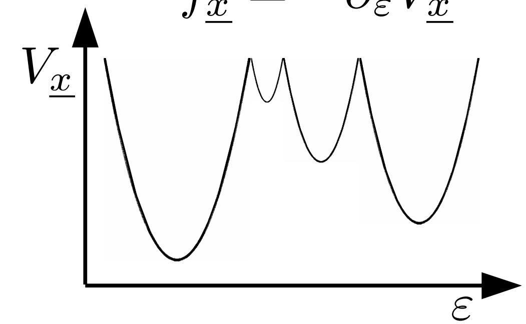
Scalar 2D model: allowing plasticity on a strain component

$$E_{\text{elast.}} = \int d^2\mathbf{r}\left(B\varepsilon_1^2 + \mu\varepsilon_2^2 + \mu\varepsilon_3^2\right) \longrightarrow E_{plast.} = \int d^2\mathbf{r}\left(B\varepsilon_1^2 + \mu\varepsilon_2^2 + V_{\underline{x}}[\mathbf{r}, \varepsilon_3]\right)$$

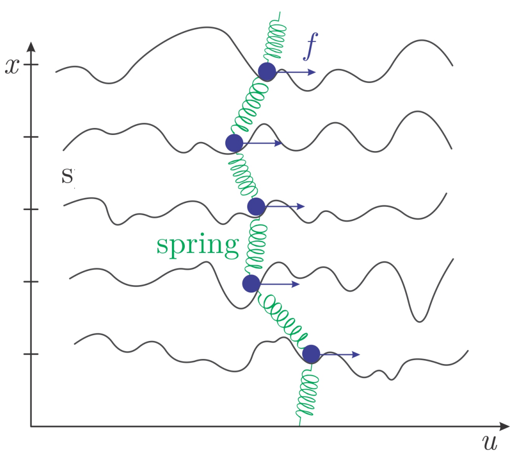
E. A. Jagla, PRE 76, 046119 (2007), PRE 101, 043004 (2020), X. Cao et al., Soft Matter 14, 3640 (2018)

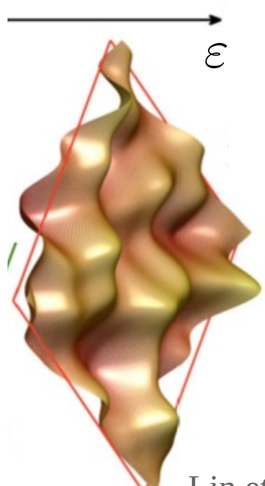
$$\partial_t \varepsilon(\mathbf{r}, t) = \underbrace{\int d^2\mathbf{r}' G(\mathbf{r} - \mathbf{r}')\varepsilon(\mathbf{r}')}_{\text{“Eshelby” interaction}} + \underbrace{f_{\underline{x}}(\mathbf{r}, \varepsilon)}_{\text{pinning force}} + \underbrace{\Sigma_{\text{ext}}}_{\text{applied stress}}$$

$$f_{\underline{x}} = -\partial_\varepsilon V_{\underline{x}}$$



Each site w/ **independent disordered potential**





Lin et al. PNAS ‘14

By construction: dynamical disorder, **no memory**

once a local strain overcomes a barrier of the parabolic basin, **the basin changes** irreversibly

Not quenched!

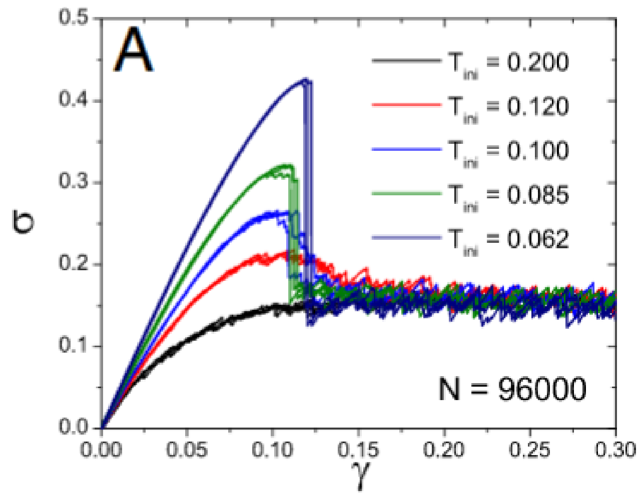
To control the macroscopic strain we use

$$\Sigma_{\text{ext}} \equiv \kappa(\gamma - \overline{\varepsilon})$$

Like the “elastic line”, but in 2D w/Eshelby-like interactions

The initial configuration

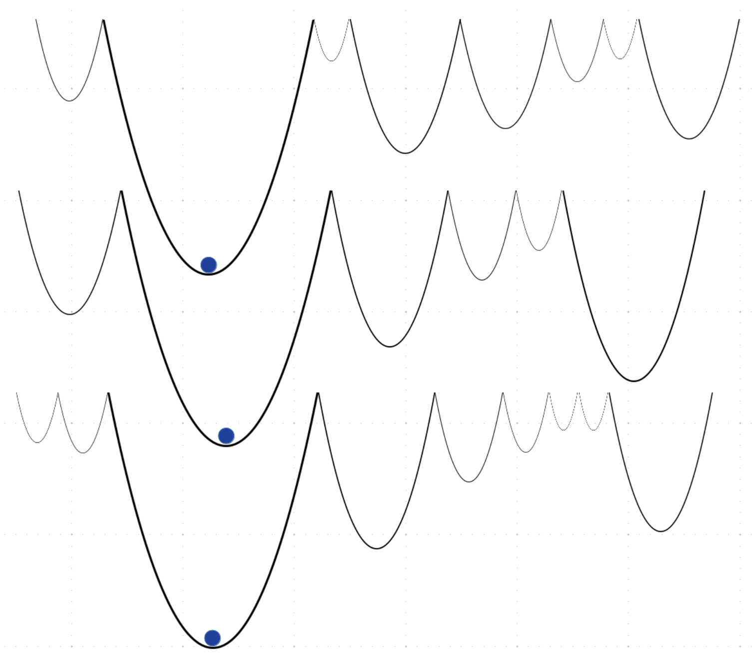
From MD we know: stress overshoot, yield stress and strain **depends on sample preparation**



Ozawa et al. PNAS **115**, 6656 (2018)

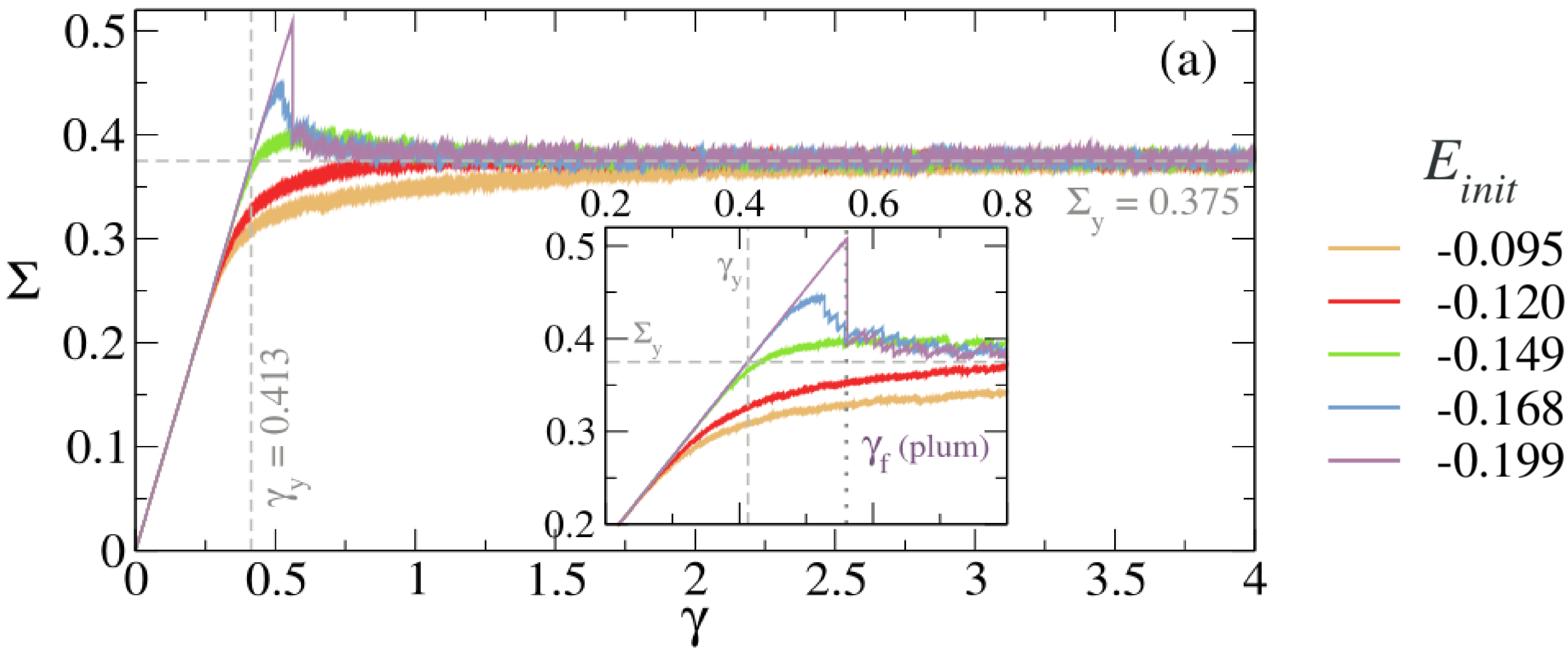
"Ductile yielding" vs. "Fragile yielding"

We **'mimic'** different degrees of annealing by starting from a highly-sheared sample and transforming its sitting wells



E_{init} decreases as we make deeper and align the wells

Uniform (quasistatic) deformation: steady liquid

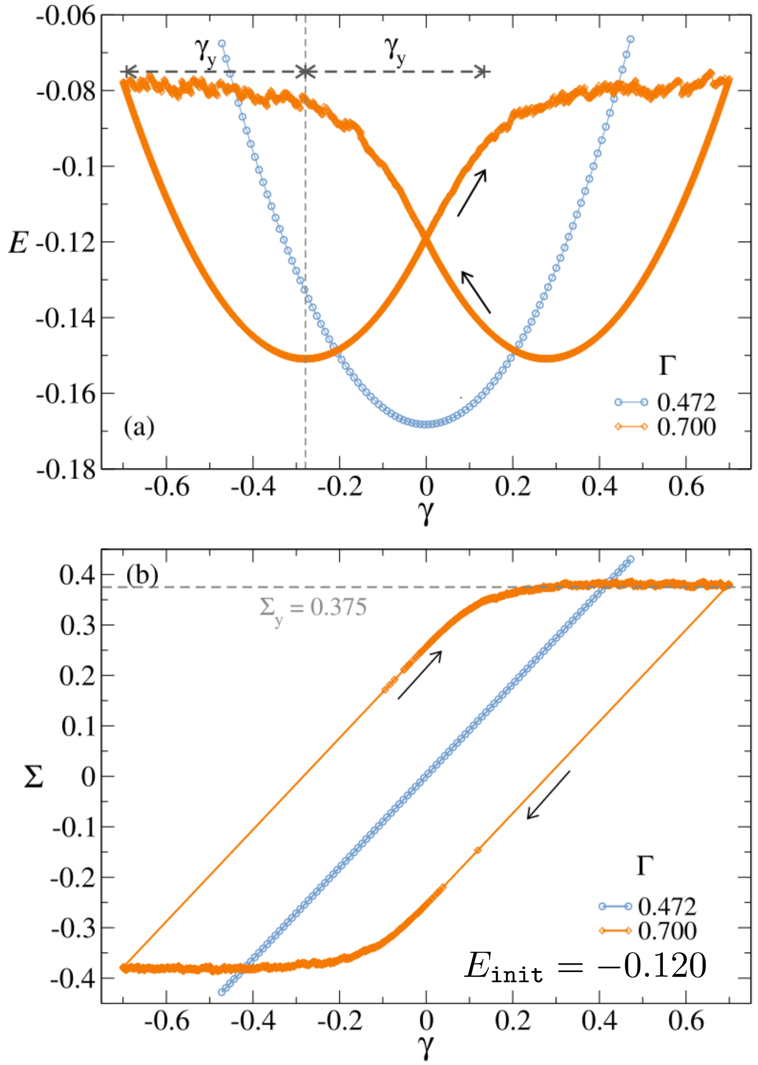


Plasticity becomes important at $$\gamma_y = \Sigma_y / \mathcal{G} \simeq 0.413$$

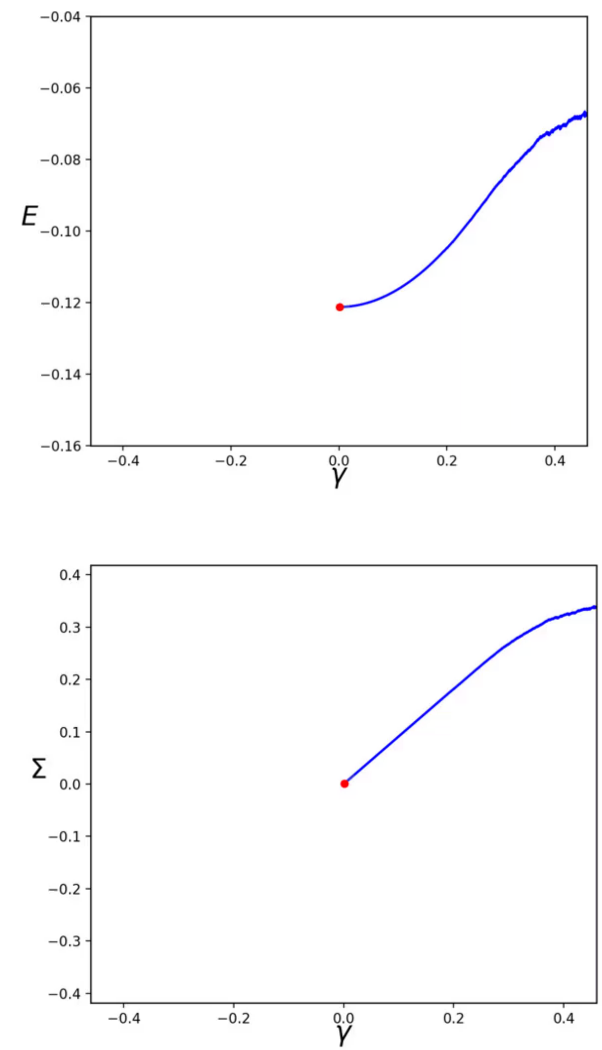
Oscillatory deformation: 2 steady phases

Starting at γ=0 we deform (quasistatically) up to +Γ, then to -Γ, then back 0, and so on...

Two steady-states: solid phase (Γ < Γc), mixed phase (Γ > Γc)



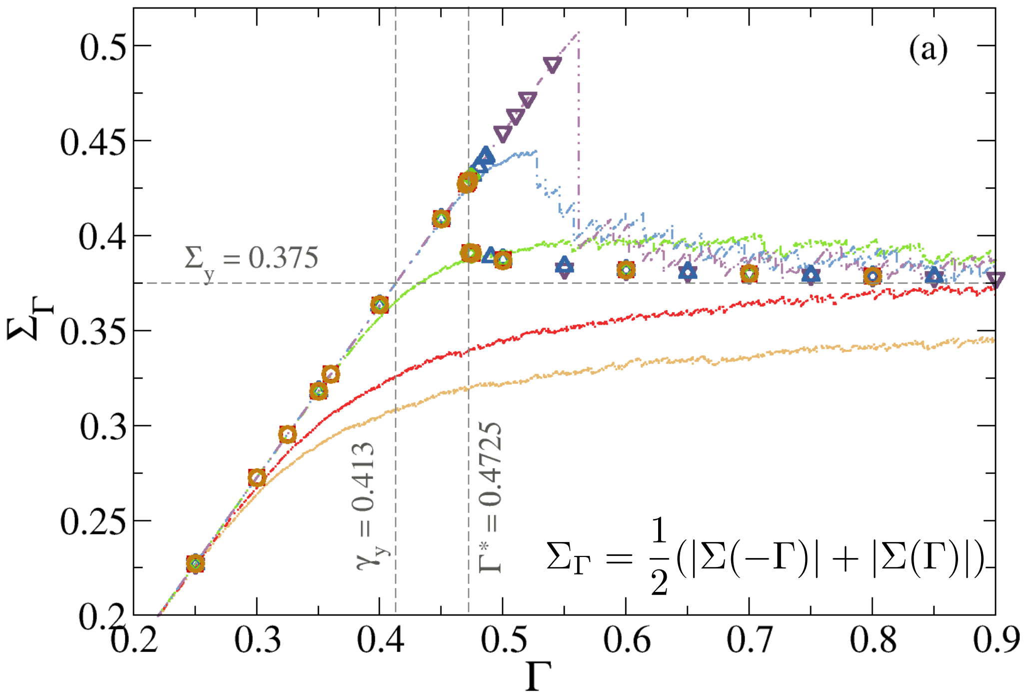
Steady state



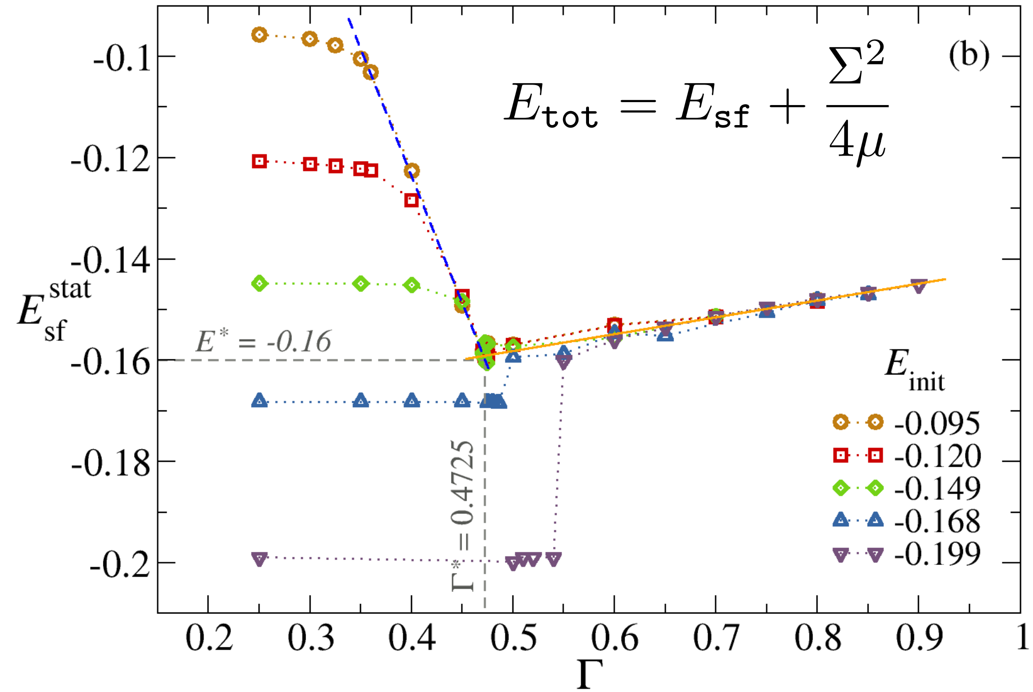
Transient evolution $\Gamma = 0.45 < \Gamma_c$

Steady stress and energy show sharp jumps

Stress at maximum strain



Per-site "**stress-free**" energy



Sharp stress jump at a critical amplitude $\Gamma_c(E_{init})$

If $(E_{\texttt{init}} > E^*) \longrightarrow \Gamma_c(E_{\texttt{init}}) = \Gamma^*$

"critical annealing level"

Above $\Gamma_c(E_{init})$, the stress of all samples is indistinguishable from Σ_y (uniform deformation)

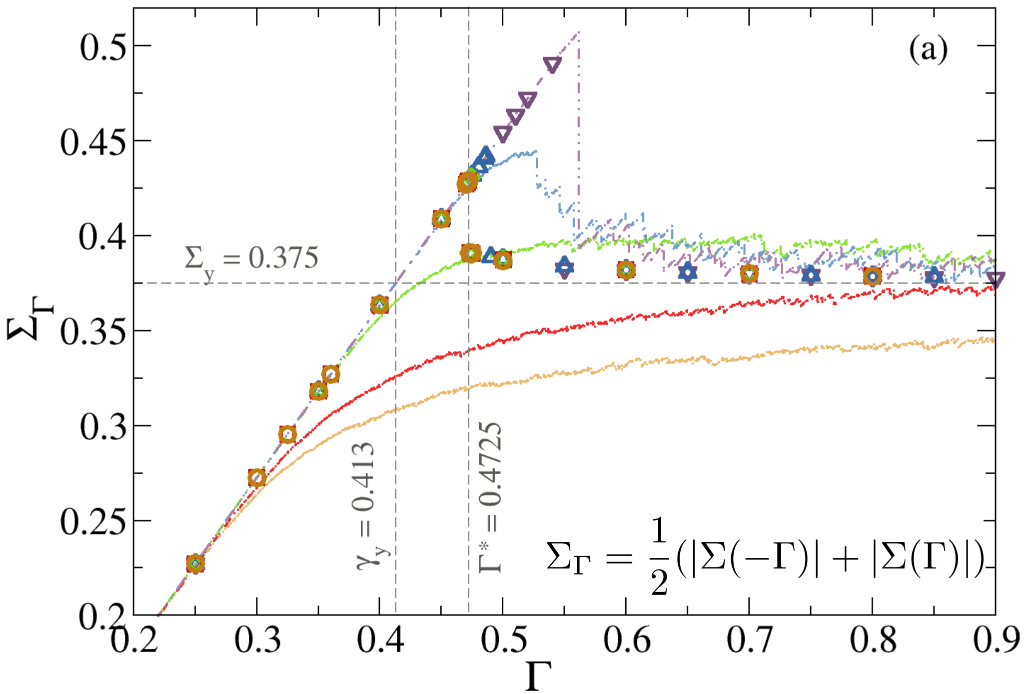
For very small Γ, E_{sf} strongly depends on E_{init}

Increasing Γ within the solid phase ($\Gamma<\Gamma_c$):

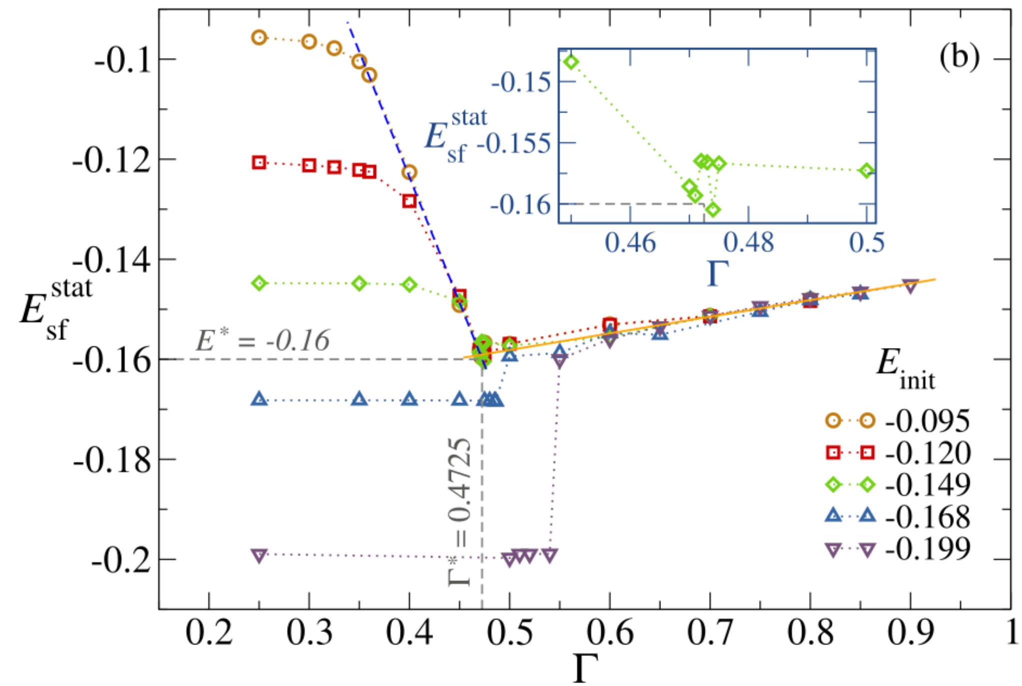
- Samples with $E_{init}<E^*$=-0.16 **keep memory**
- Samples with $E_{init}>E^*$ **shear anneal**

Steady stress and energy show sharp jumps

Stress at maximum strain



Per-site “**stress-free**” energy



Sharp stress jump at a critical amplitude $\Gamma_c(E_{init})$

If $(E_{\texttt{init}} > E^*)$ ⟶ $\Gamma_c(E_{\texttt{init}}) = \Gamma^*$

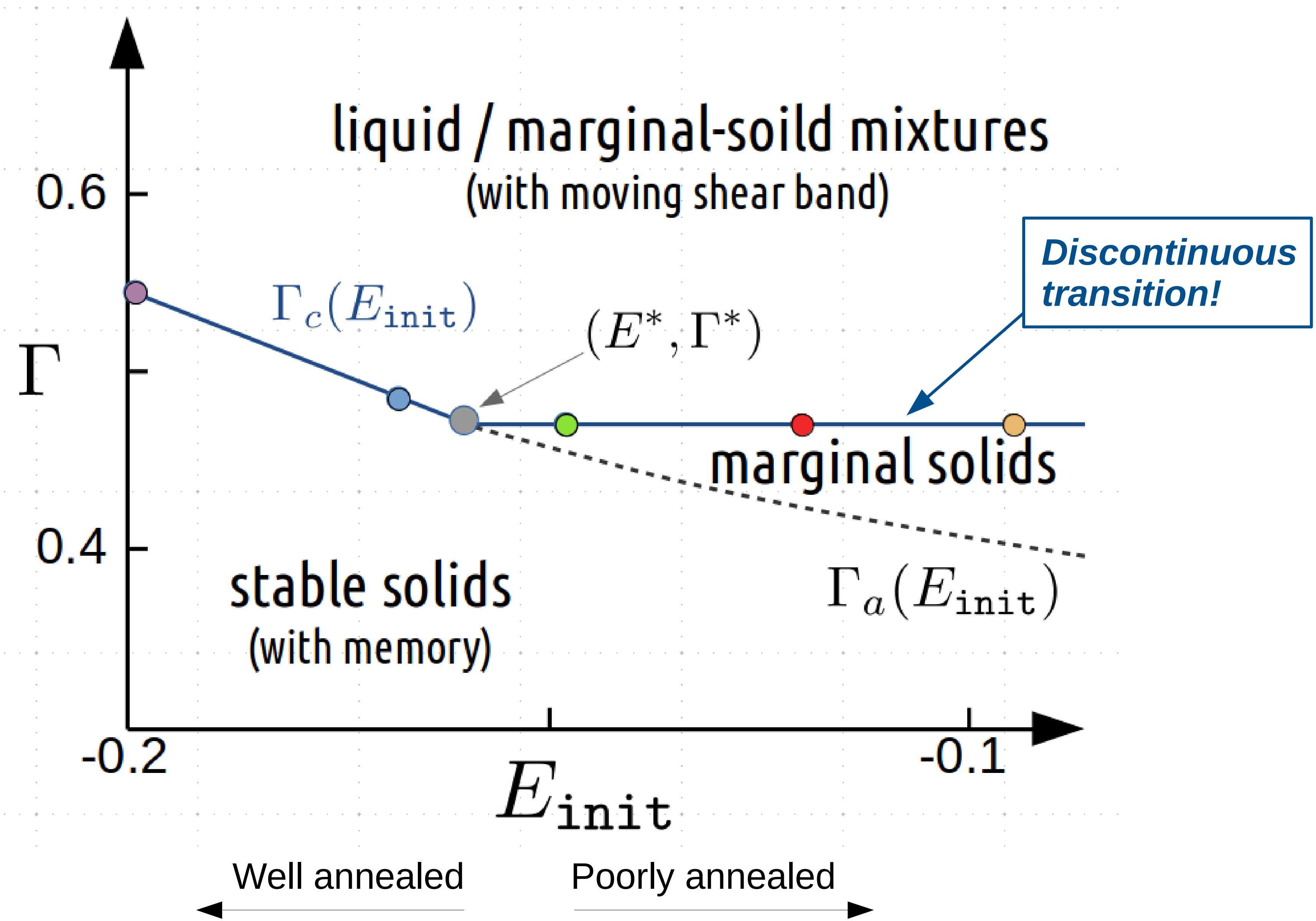
“critical annealing level”

Above $\Gamma_c(E_{init})$, the stress of all samples is indistinguishable from Σ_y (uniform deformation)

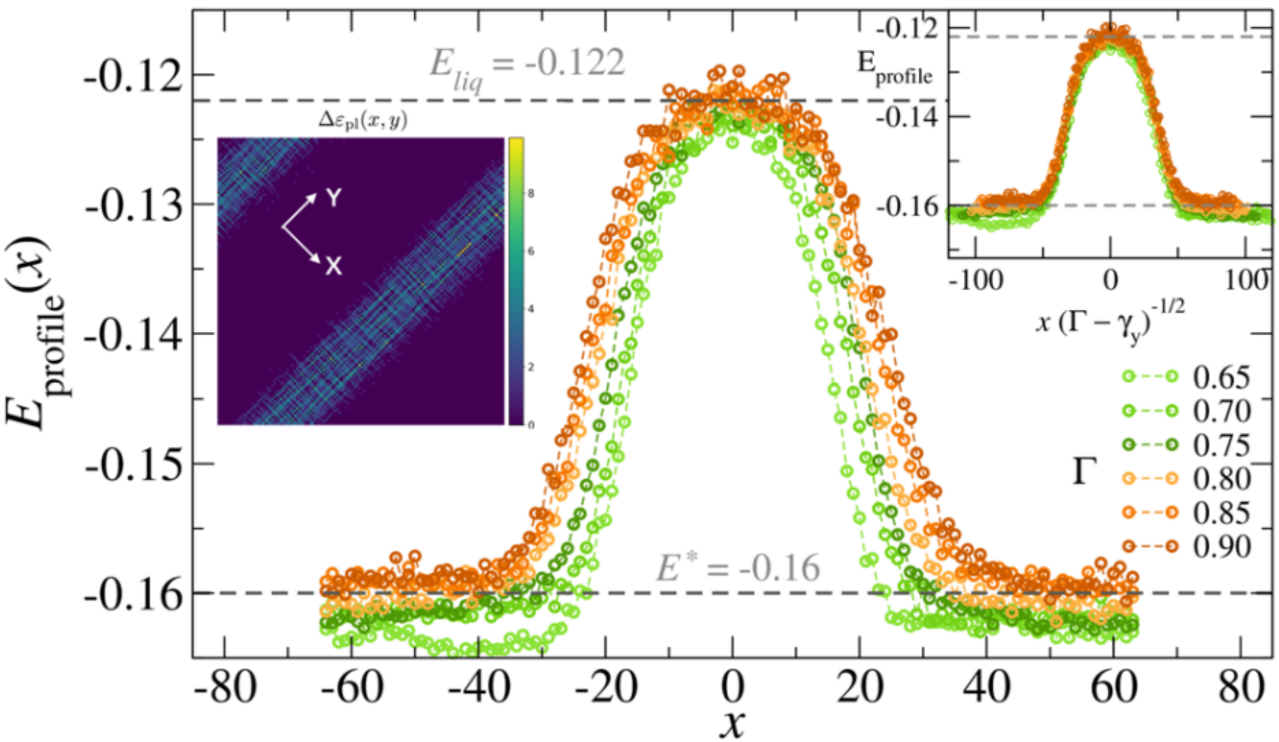
Even when it’s less evident, the **energy E_{sf} also has a discrete jump** at the transition

Finally, $\boldsymbol{E_{sf}}$ **grows with $\boldsymbol{\Gamma}$** (orange line)

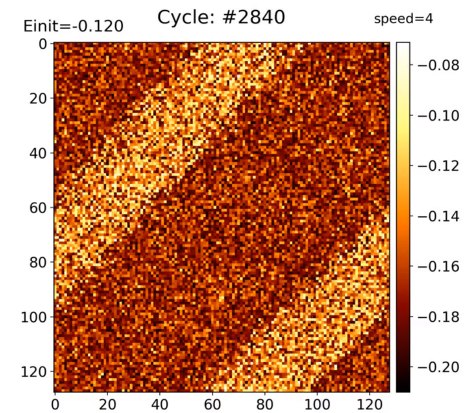
Steady-state: “Phase diagram”



Mixed state at $\Gamma > \Gamma_c$: fluid band + marginal solid



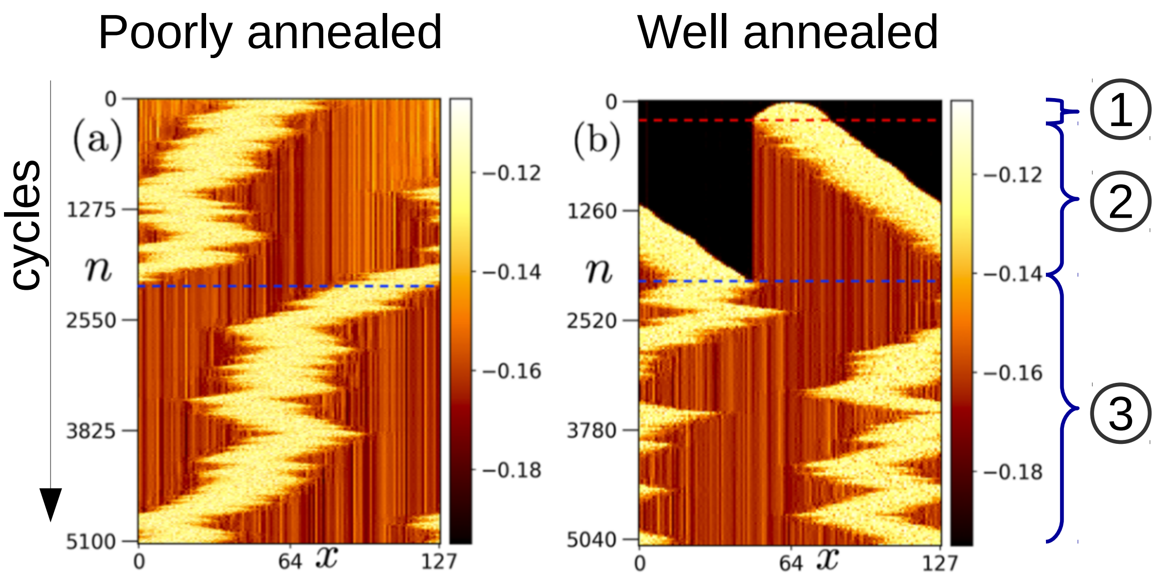
stroboscopic video



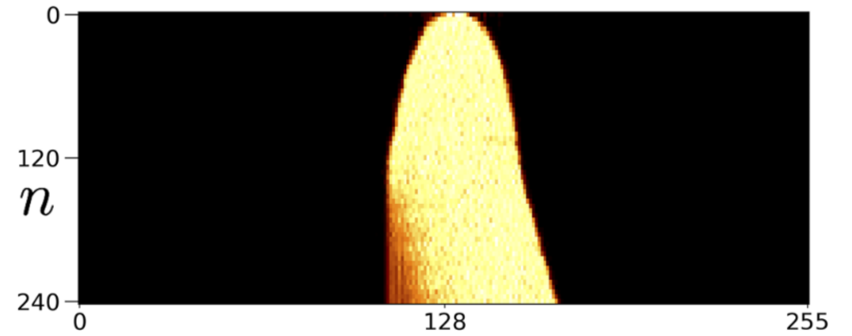
color: local energy

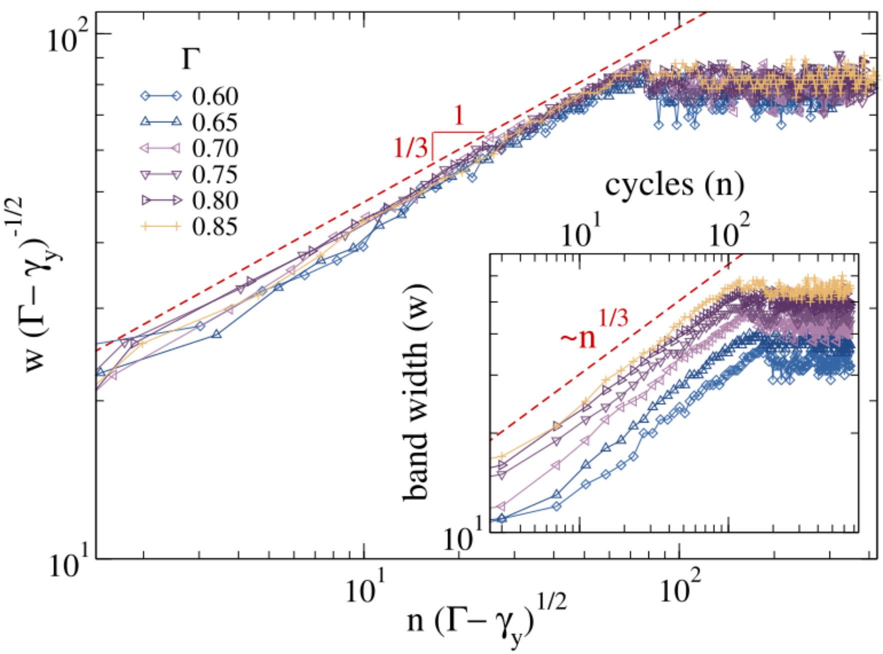
- **Center of the band** has the same energy as the **fluid** state in uniform deformation E_{liq}
- **Outside** the band the system is mostly at the **marginal solid** state E^*
- Band-**width increases** as $w_s \sim (\Gamma - \Gamma_0)^{1/2}$, *with* $\Gamma_0 = \gamma_y$.
- Notice that $\gamma_y < \Gamma^* \leq \Gamma_c$. So, **at the transition the band is finite**: $w_s(\Gamma_c) > 0$

Transient (at $\Gamma>\Gamma_c$): various dynamical stages



x: band-trasverse coordinate; color: local energy



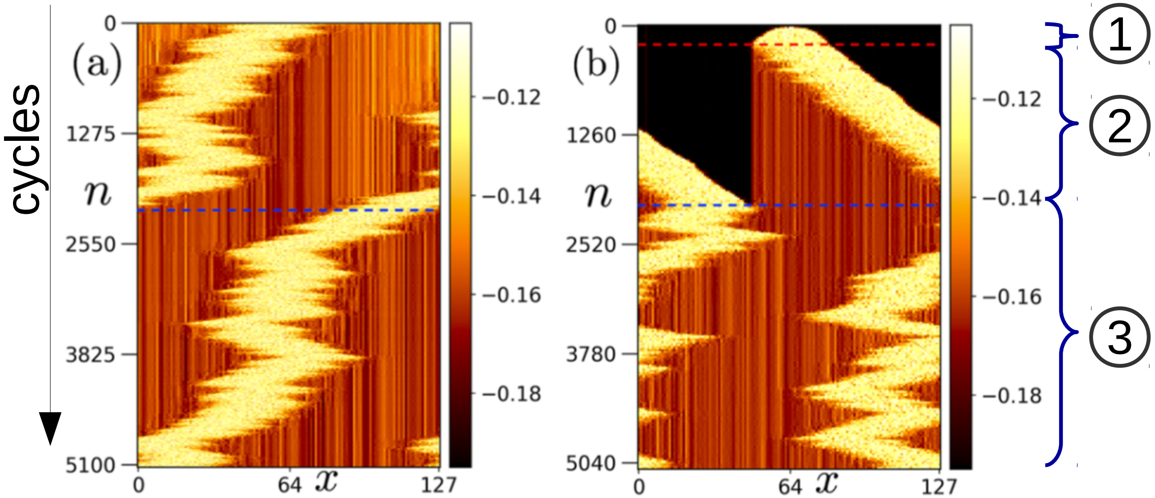


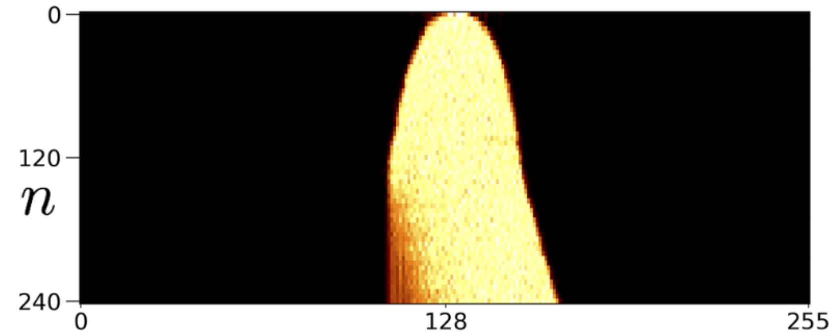
1) Band emergence and **coarsening**

2) Ballistic **swipe out** of deeply annealed region

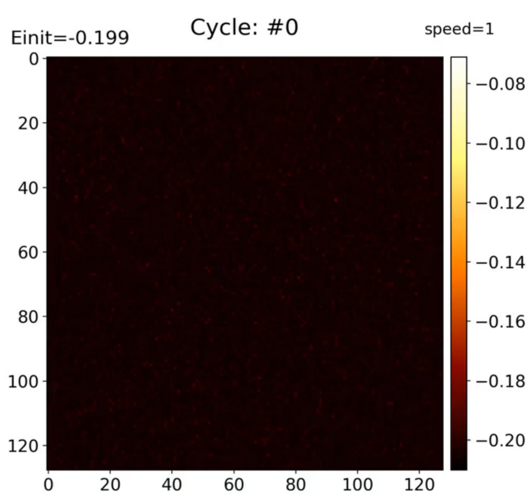
Transient (at $\Gamma > \Gamma_c$): various dynamical stages

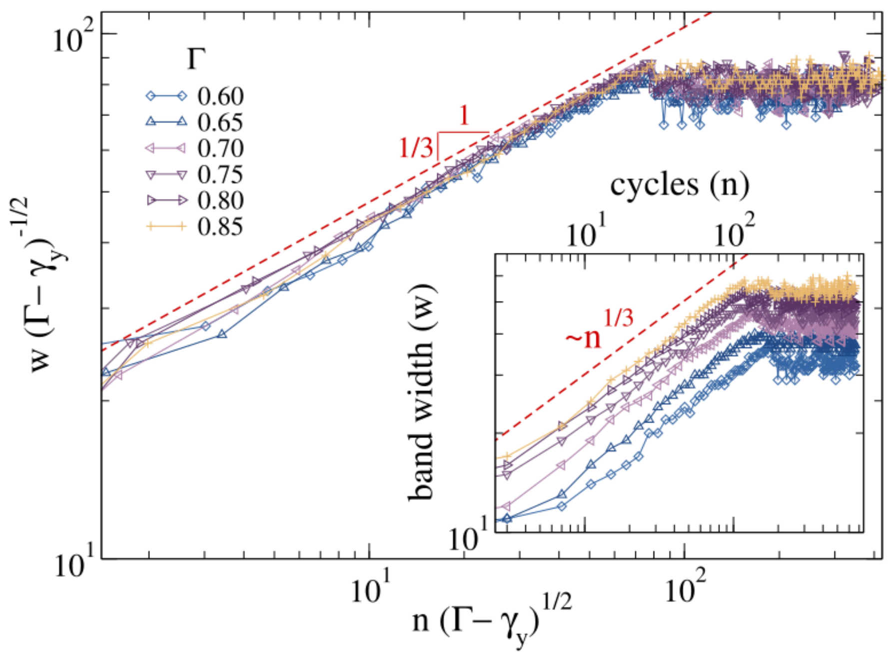
Poorly annealed — Well annealed





x: band-trasverse coordinate; color: local energy





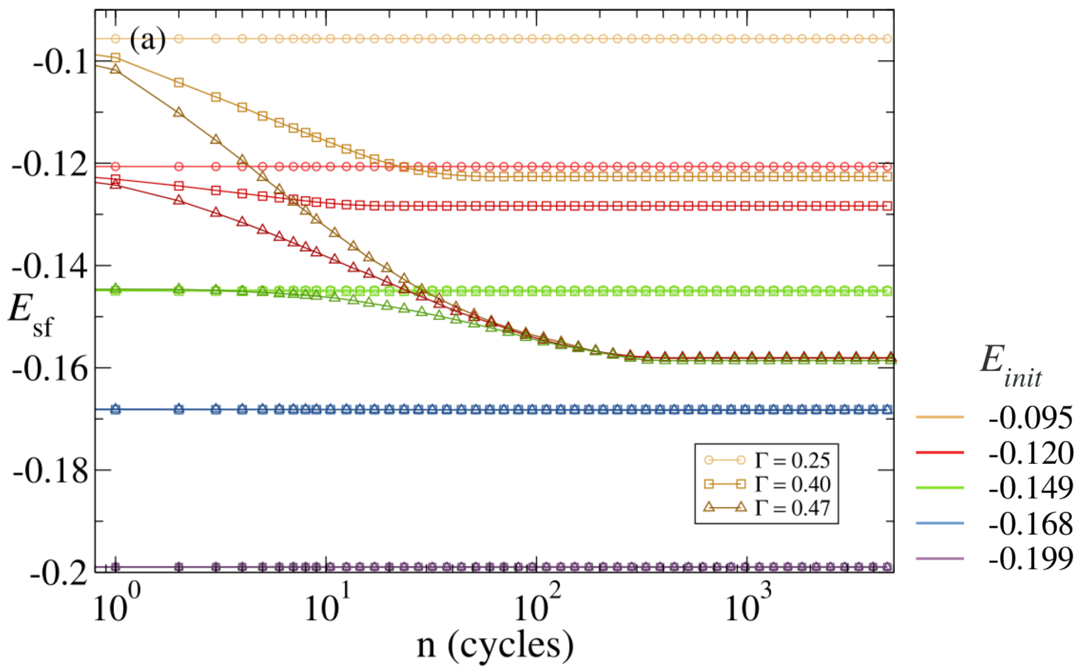
1) Band emergence and **coarsening**

2) Ballistic **swipe out** of deeply annealed region

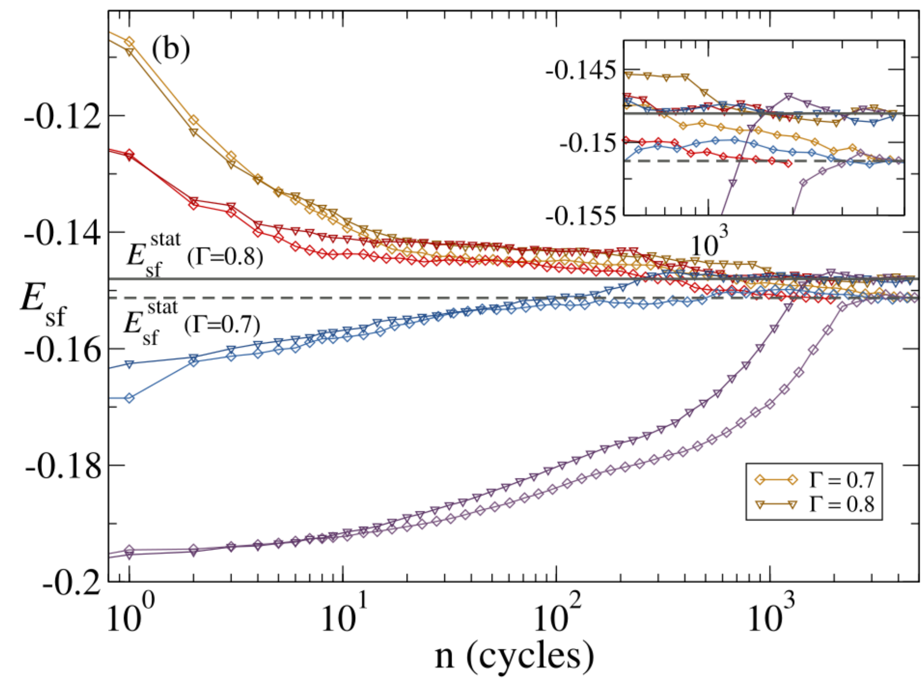
3) Anomalous **diffusion**

Transient behavior

$\Gamma < \Gamma_c$



$\Gamma > \Gamma_c$



Ultra-stable systems (E_{init}<E^*) are **unperturbed** by the oscillations

Systems with E_{init}>E^* **shear-anneal** (transient annealing!) if the amplitude is large enough

Notice all three poorly annealed samples coming together to the same steady-state for $\Gamma_a<\Gamma=0.47<\Gamma_c$

Above Γ_c, all samples go to **the same** (Γ-dependent) **stationary state at large *n***

The stationary E_{sf} grows with Γ, as the liquid **shear-band** of the mixed phase **gets wider and wider**

Thanks!

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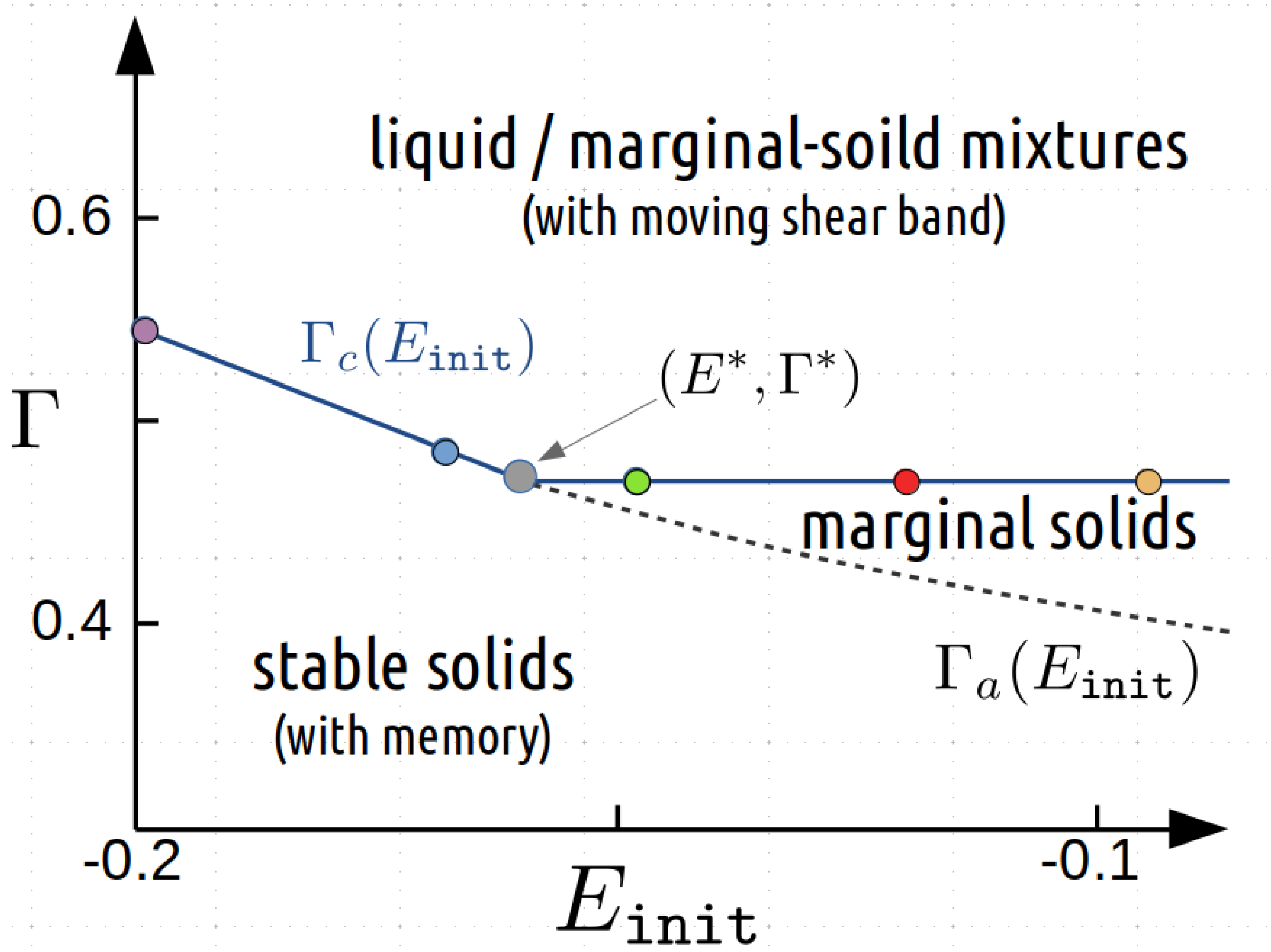

Have a look to ...

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Open questions/paths

- Are there transient states of **multiple** shear-bands in very large systems? How do they merge (or not) in a single band in the steady-state?

- If we set-up a **hierarchical disorder** with memory at small scales and no-memory at the meta-basin scale, do we recover the full atomistic simulations picture (including “revesible” plastic events)?

- How does the **critical annealing level E*** detected in the oscillatory protocol compares to annealing temperatures that distinguishing between **ductile and brittle** yielding in uniform shear deformation?

- How do we explain the **ballistic motion** of the shear band observed for initially very deeply annealed systems?