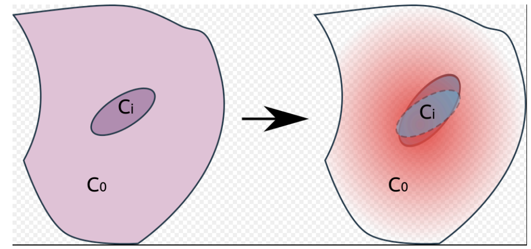
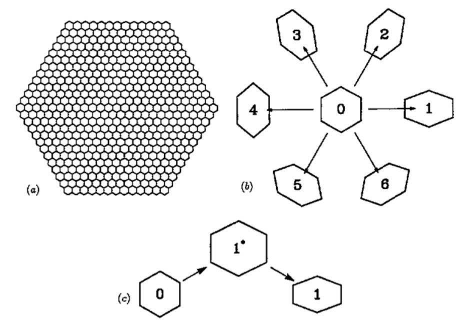
Elasto-plastic models: ingredients

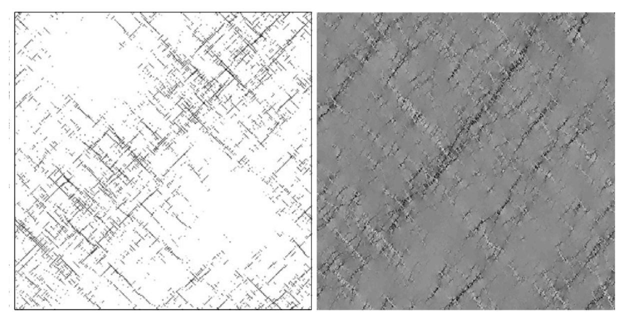
- State description / yielding criterion
  - Eshelby?
  - Compatibility of strain?
  - Near field vs. far field?
  - Elastic heterogeneity allowed/included?

- Stochasticity
  - Quenched disorder?
  - Dynamically generated threshold conditions?
  - Dynamical equations deterministic or stochastic?

- Dynamical evolution
  - Deterministic vs. stochastic?
  - Inertia?
  - Damping?
  - If stochastic, which degrees of freedom does the noise act on?

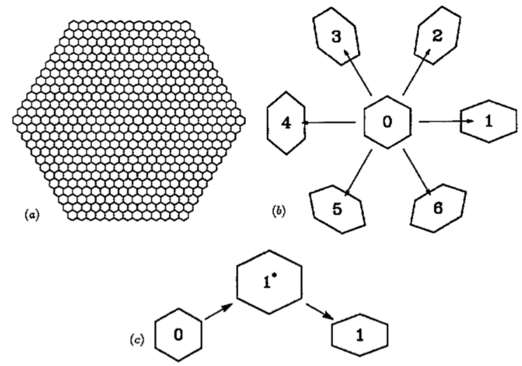






Elasto-plastic models: recipes

- Bulatov and Argon (Mod. Sim. Mat. Sci&Eng 1994)
  - Homer, Rodney and Schuh
- Baret, Vandembroucq and Roux (PRL 2002)
  - Talamali, Vandembroucq, and Roux
  - Budrikis and Zapperi
  - Lin, Lerner, Rosso and Wyart
- Onuki (PRE 2003)
- Picard, Ajdari and Bocquet (PRE 2005)
  - Barrat, Martens, Nicolas, Ferrero...
- Jagla (PRE 2007)

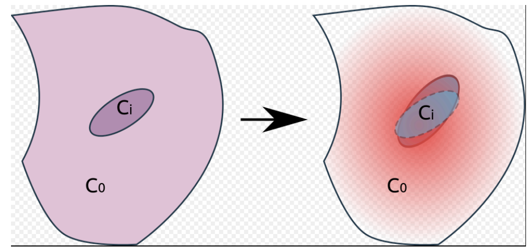


Elasto-plastic models: recipes

	Primary DOF	Landscape / Barriers	Dynamics
Bulatov	ε-plastic (integer)	Uniform Thresholds	kMC
Onuki	displacement (continuous)	Uniform Thresholds	Langevin
Baret / Talamali	ε-plastic (integer)	Redrawn Thresholds	Extremal
Picard / Martens	ε-plastic (integer)	Uniform Thresholds	Threshold+Poisson
Jagla	total strain (continuous)	Quenched Disorder	Langevin + “Relaxation”

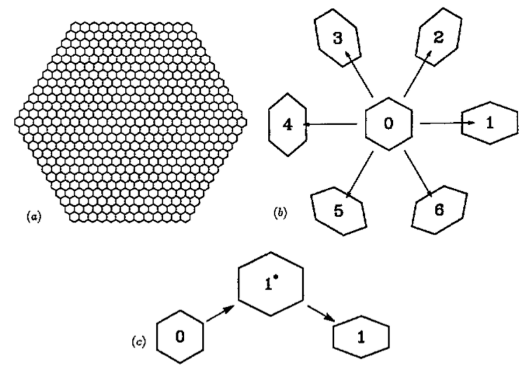
Bulatov and Argon (Mod. Sim. 1994)

	Primary DOF	Landscape / Barriers	Dynamics
Bulatov	ε-plastic (integer)	Uniform Thresholds	kMC



- Explicit Eshelby description of plastic transformation:
  - Space is tiled.
  - Any tile may undergo plasticity
  - Reference strain incremented in one of six eigenstrains.
  - Stress (elastic strain) computed via Eshelby
  - Need to assume small deformations

- Dynamics:
  - kinetic Monte Carlo
  - $w(n,\alpha) = \omega_0 \exp\left\{-\left[\Delta F_0 - \Omega\langle\sigma_{ij}(n,t)\rangle e^*_{ij}(\alpha)\right]/kT\right\}$
  - ω is the rate for the n-th tile to make the α-th transition
  - e* is a transitory state including some dilation
  - $\sigma_{ij}(n,t)$ is the stress at the n-th tile calculated from global load and all other previous plastic transformations.
  - $\omega_0 \exp[-\Delta F_0/kT]$: spontaneous, unbiased transformation rate



- Disorder:
  - Plastic strain increment fixed
  - Initial stresses before loading either:
    - homogeneous (if no initial plasticity) or
    - disordered (if initial plasticity)

Bulatov and Argon (Mod. Sim. 1994)

	Primary DOF	Landscape / Barriers	Dynamics
Bulatov	ε-plastic (integer)	Uniform Thresholds	kMC

Total citations Cited by 113

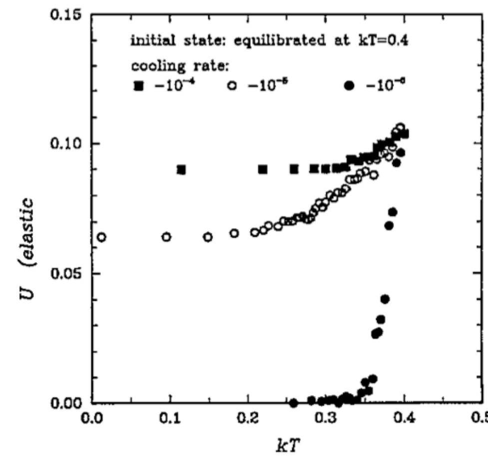
Scholar articles A stochastic model for continuum elasto-plastic behavior. I. Numerical approach and strain localization
VV Bulatov, AS Argon - Modelling and Simulation in Materials Science and . . ., 1994
Cited by 113 - Related articles - All 2 versions

- No citations for first 5 years!
- First non-self-citation from Falk and Langer review in MRS Bulletin 2000

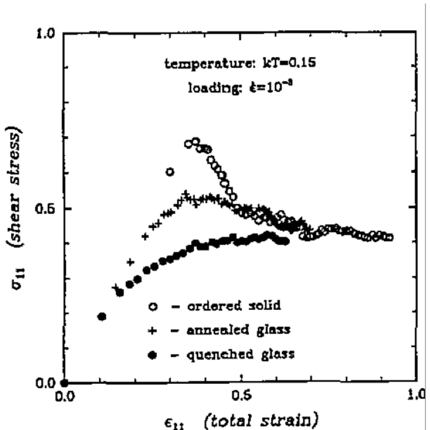
Bulatov and Argon (Mod. Sim. 1994)

	Primary DOF	Landscape / Barriers	Dynamics
Bulatov	ε-plastic (integer)	Uniform Thresholds	kMC

- No loading (paper II):
  - “Glass transition”
  - Non-exponential stress relaxation
  - Memory effects (Kovacs)



- Loading (paper III):
  - Shear localization depending on history
  - “Ordered solid”: strong overshoot/localization
  - “Quenched glass”: no overshoot, (transient localization?)
  - “Annealed glass”: mild overshoot/localization



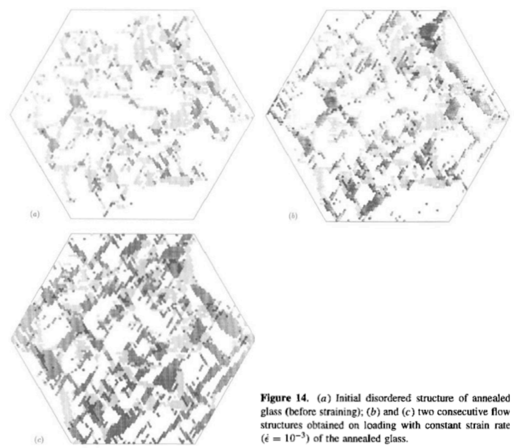
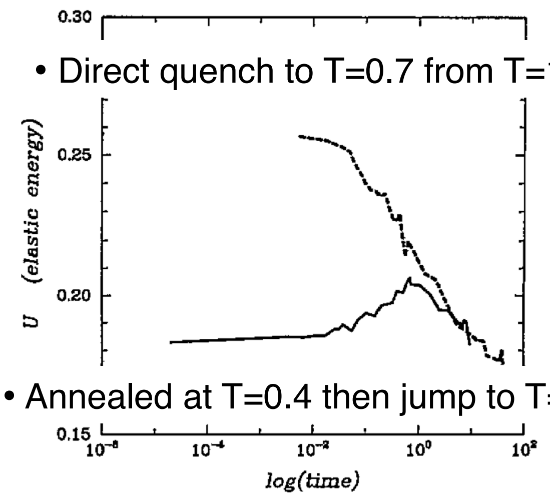
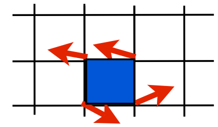


Figure 14. (*a*) Initial disordered structure of annealed glass (before straining); (*b*) and (*c*) two consecutive flow structures obtained on loading with constant strain rate ($\dot{\epsilon} = 10^{-3}$) of the annealed glass.



- Direct quench to T=0.7 from T=1.0
- Annealed at T=0.4 then jump to T=0.7

Onuki (PRE 2003)



	Primary DOF	Landscape / Barriers	Dynamics
Onuki	displacement (continuous)	Uniform Thresholds	Langevin

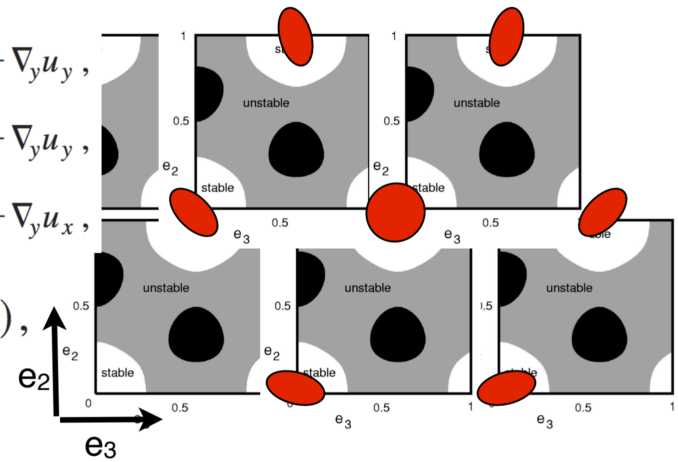
- "Implicit Eshelby"
  - Displacements / strains on square lattice
  - Local free energy density is simple, non-convex, periodic function of shear strain (Frenkel model)
  - Transformation symmetries identical to Bulatov
  - Lattice different from Bulatov

$$e_1 = \nabla_x u_x + \nabla_y u_y ,$$

$$e_2 = \nabla_x u_x - \nabla_y u_y ,$$

$$e_3 = \nabla_x u_y + \nabla_y u_x ,$$

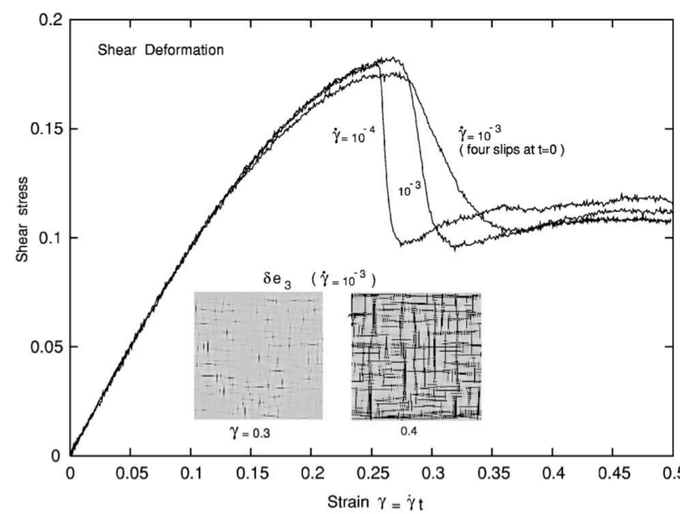
$$f_{\rm el} = \tfrac{1}{2} K_0 e_1^2 + \mu_0 \Phi(e_3', e_2'),$$



$$\rho \frac{\partial}{\partial t} \boldsymbol{v} = \boldsymbol{\nabla} \cdot \overleftrightarrow{\sigma} + \eta_0 \nabla^2 v + \boldsymbol{\nabla} \cdot \overleftrightarrow{\sigma}_{\rm R} ,$$

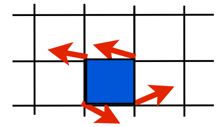
$$\langle \sigma_{ij}^{\rm R}(\boldsymbol{r},t) \sigma_{ij}^{\rm R}(\boldsymbol{r}',t') \rangle = 2 k_{\rm B} T \eta_0 \delta(\boldsymbol{r}-\boldsymbol{r}') \delta(t-t')$$

- Stresses and dynamics:
  - $\sigma = \delta f_{el} / \delta \varepsilon$
  - η_0Grad[v]: Viscous stress
  - σ_R: Langevin driving via random stress, (not force)
  - Accelerations from: div[elastic+viscous+random]



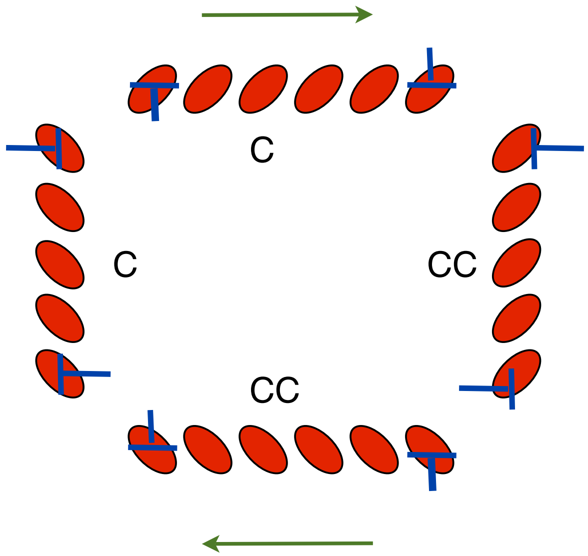
•Eshelby transformation field comes "for free" from elasticity... legitimate? (i.e. sensitive to discretization?)

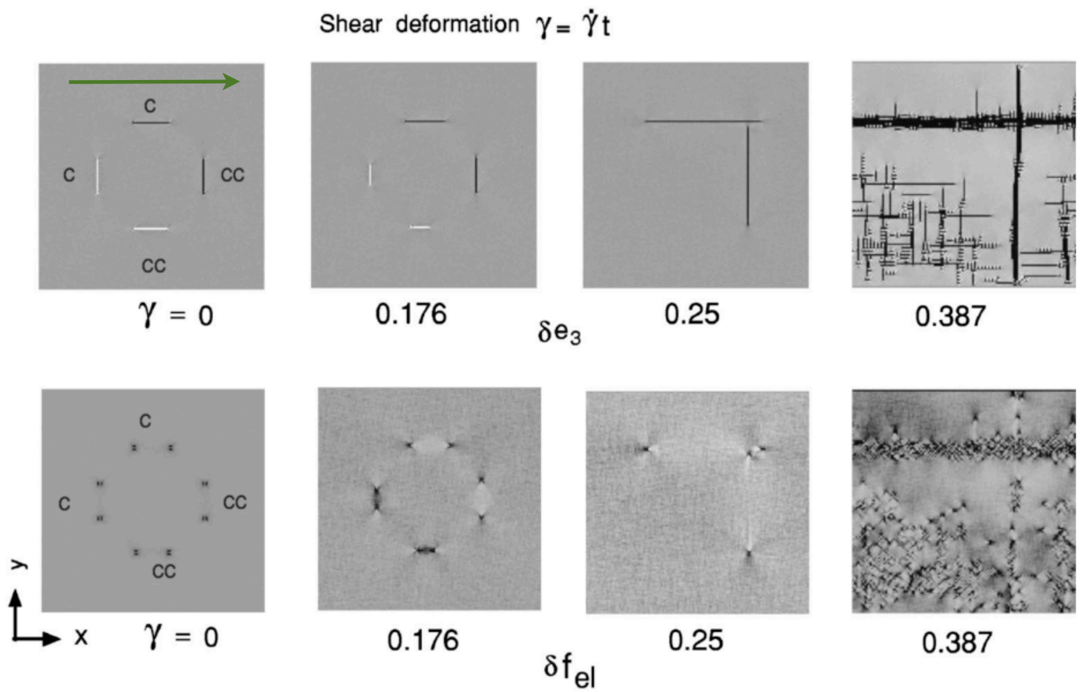
Onuki (PRE 2003)



	Primary DOF	Landscape / Barriers	Dynamics
Onuki	displacement (continuous)	Uniform Thresholds	Langevin

- Seeds with four “slips”
- C:Clockwise and CC: Counterclockwise

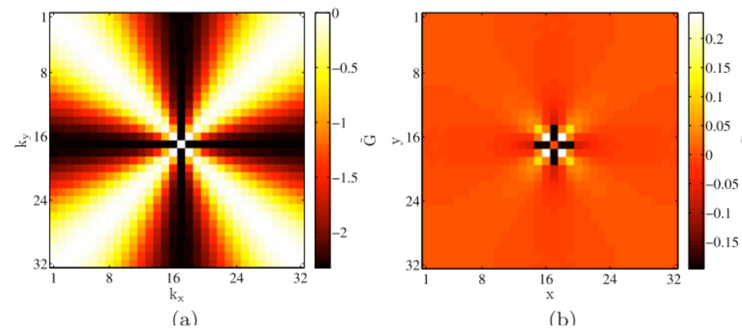


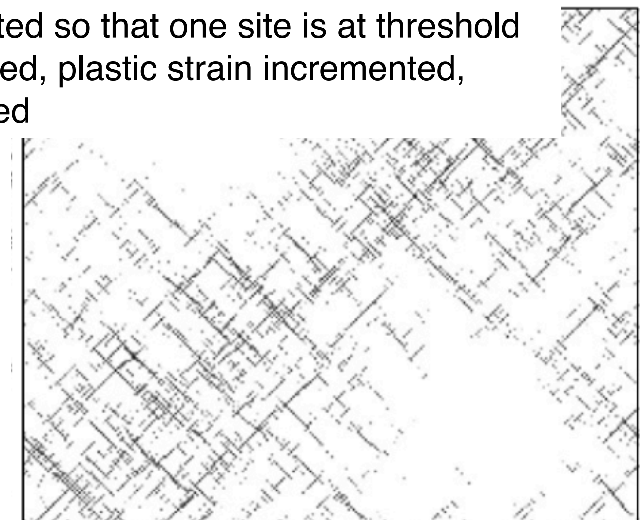


Talamali et. al. (Compt. Rend. Mech. 2012)

	Primary DOF	Landscape / Barriers	Dynamics
Baret / Talamali	ε-plastic (integer)	Redrawn Thresholds	Extremal

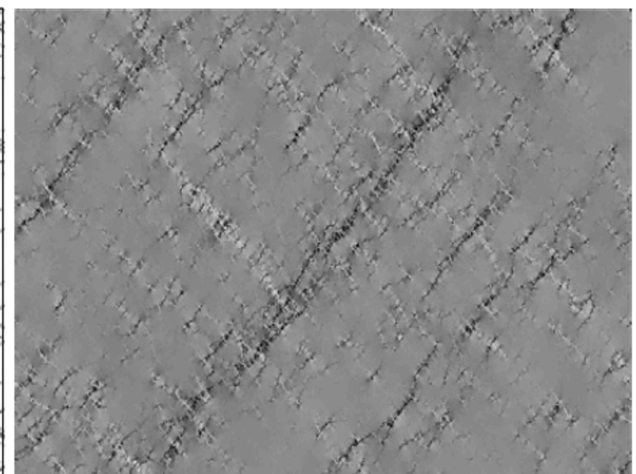
- Explicit Eshelby (but far field only)
  - Plastic transformation redistributes stresses
  - Kernel from far-field Eshelby.
  - Discretized and truncated in Fourier space
  - Plastic strain amplitude, “d/a”, uniform
  - Plastic strain orientation aligned with global loading
- Extremal dynamics:
  - Local threshold stress chosen from a distribution
  - Global load adjusted so that one site is at threshold
  - Stress is transferred, plastic strain incremented, stress is redistributed





- Extremal model, L=256, $\Delta\varepsilon_{plastic}$=0.01
- Talamali et. al. Compt. Rend. 2012

(b)



- MD (2D Lennard-Jones) simulation, L=1000, $\Delta\varepsilon_{plastic}$=0.04
- CM and Mark Robbins. PRL 2008

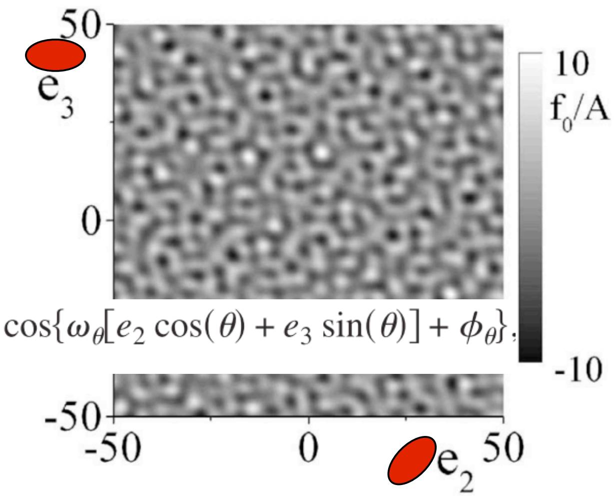
(c)

Jagla (PRE 2007)

	Primary DOF	Landscape / Barriers	Dynamics
Jagla	total strain (continuous)	Quenched Disorder	Langevin + “Relaxation”

- “Implicit Eshelby” similar to Onuki
  - Strains on square lattice
  - Compatibility (Saint-Venant) imposed on the side
  - Local f generated from random waves
  - Barriers and possible transformations disordered

$$e_1 = \nabla_x u_x + \nabla_y u_y \,,$$
$$e_2 = \nabla_x u_x - \nabla_y u_y \,,$$
$$e_3 = \nabla_x u_y + \nabla_y u_x \,,$$



$$f_0(e_2,e_3) = A\sum_\theta \cos\{\omega_\theta[e_2\cos(\theta) + e_3\sin(\theta)] + \phi_\theta\},$$

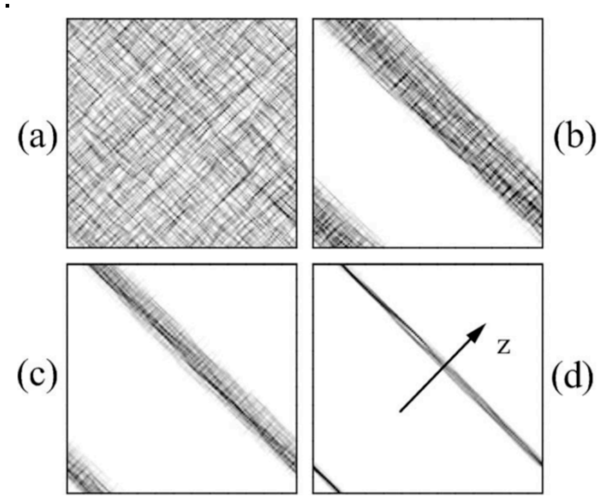
- Dynamics:
  - Gradient dynamics w/compatibility

$$\frac{\partial e_i(x,y)}{\partial t} = \eta\sigma_i(x,y) + \Lambda_i(x,y,e_i,t),$$

  - “Relaxation” of strains:
    - shift e_2 and e_3 by e_2^0 and $e_3 0$
    - allow “relaxation” of e_0
    - demand compatibility on e
    - diffusion of stress

$$f_0(e_2,e_3) \to f_0(e_2 - e_2^0, e_3 - e_3^0)$$
$$\frac{\partial e_i^0(x,y)}{\partial t} = \lambda\nabla^2 \frac{\delta F}{\delta e_i^0(x,y)}$$

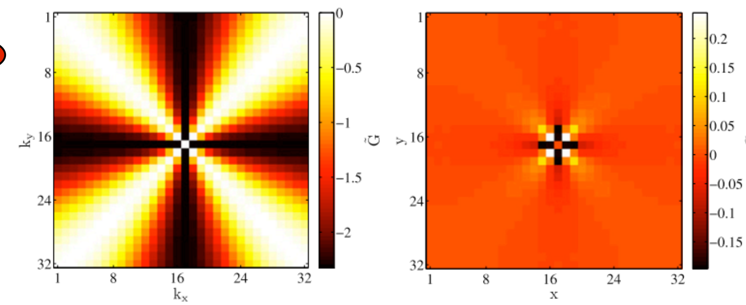
- Localization enhanced by:
  - shearing slower
  - or waiting longer



Picard et. al. (PRE 2005)

	Primary DOF	Landscape / Barriers	Dynamics
Picard / Martens	ε-plastic (integer)	Uniform Thresholds	Threshold+Poisson

- Similar to Baret, but...
  - Threshold stresses are uniform
  - But yielding events occur stochastically in time
  - Initiate Poisson process above threshold
  - Recent versions: deterministic, finite rate (Ezequiel?)



(a) (b)

Questions / issues

	Primary DOF	Landscape / Barriers	Dynamics
Bulatov	ε-plastic (integer)	Uniform Thresholds	kMC
Onuki	displacement (continuous)	Uniform Thresholds	Langevin
Baret / Talamali	ε-plastic (integer)	Redrawn Thresholds	Extremal
Picard / Martens	ε-plastic (integer)	Uniform Thresholds	Threshold+Poisson
Jagla	total strain (continuous)	Quenched Disorder	Langevin + "Relaxation"

- Continuous degrees of freedom vs. automata:
  - connection to floppy modes / soft spots possible with continuous approach... fruitful?
  - number of possible transitions important?
    - Baret / Picard: n=1
    - Bulatov/Onuki: n=6
    - Jagla: n~infinity
- Dynamics:
  - dynamic vs. quenched disorder
  - Langevin on stresses rather than displacements?
  - form of the drag
  - inertia?

- Discretization of elasticity / form of stress kernel?

- What do we want to get out??? "Better" than particle-scale models?