Aging and Coarsening in Dislocation Glasses

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Aging and Coarsening in Dislocation Glasses

I. Pattern formation

II. Concepts of non-equilibrium phenomena

III. Numerical simulations of dislocations

IV. Glide, no climb: Aging, Freezing

V. Climb: Domain formation, Coarsening

VI. Wall formation: mean field, beyond mean field

VII. Role of Anchors

I. Pattern Formation

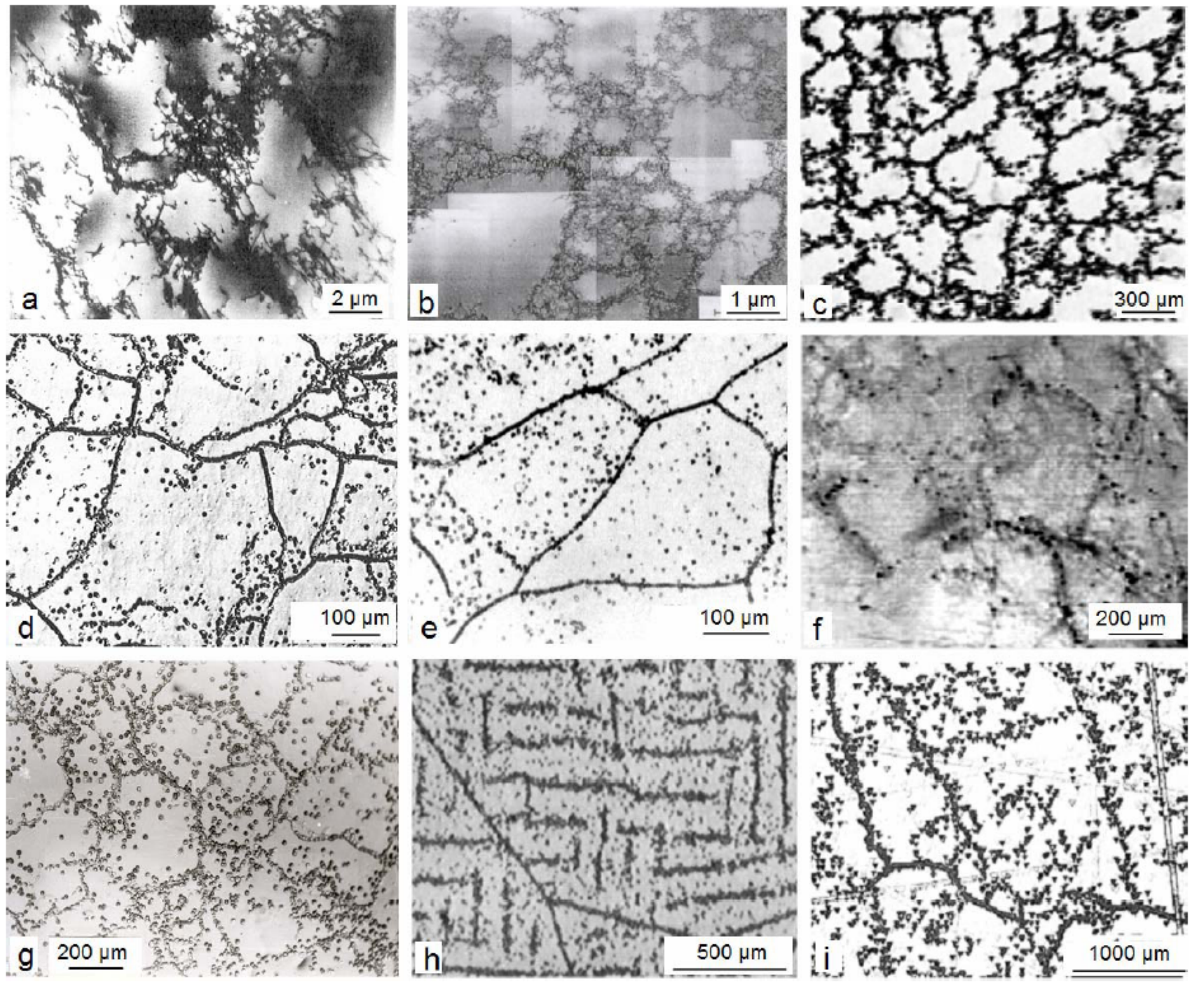


Fig. 1 Dislocation patterns formed in various crystals under differing stress conditions. (a) Mo 12% deformed at 493 K [1]; (b) Cu-Mn crystal deformed at 68.2 MPa [2]; (c) GaAs crystal grown by VCz (author's image); (d) CdTe crystal grown by VB (authors image); (e) PbTe crystal grown by VB [33]; (f) SiC crystal grown by sublimation (courtesy of D. Siche from IKZ Berlin); (g) $Cd_{0.96}Zn_{0.04}Te$ crystal grown by VB (author's image); (h) NaCl crystal with labyrinth structure deformed by 150 MPa at $T/T_m = 0.75$ [3], (i) CaF_2 crystal grown by VB [4].

I. Pattern Formation

Pattern formation in dislocation systems is ubiquitous

Equilibrium statistical physics: low T phase is dilute gas of dislocations with density vanishing as $T \to 0$

Pattern formation is a far from equilibrium phenomenon

I. Pattern Formation

Early approaches

1. Rate equations (Kocks)

2. Mobile and immobile dislocations, transitions between (Kubin)

3. Intersecting dislocation loops (Friedel, Kubin)

4. Reverse diffusion (Holt)

5. Forward Diffusion + Two types of dislocations (Walgraef-Aifantis)

6. Statistical ensembles (Ananthakrishna)

II. Concepts of Non-equilibrium Dynamics

Start system far out of equilibrium, let it relax

Three hallmarks of glassiness

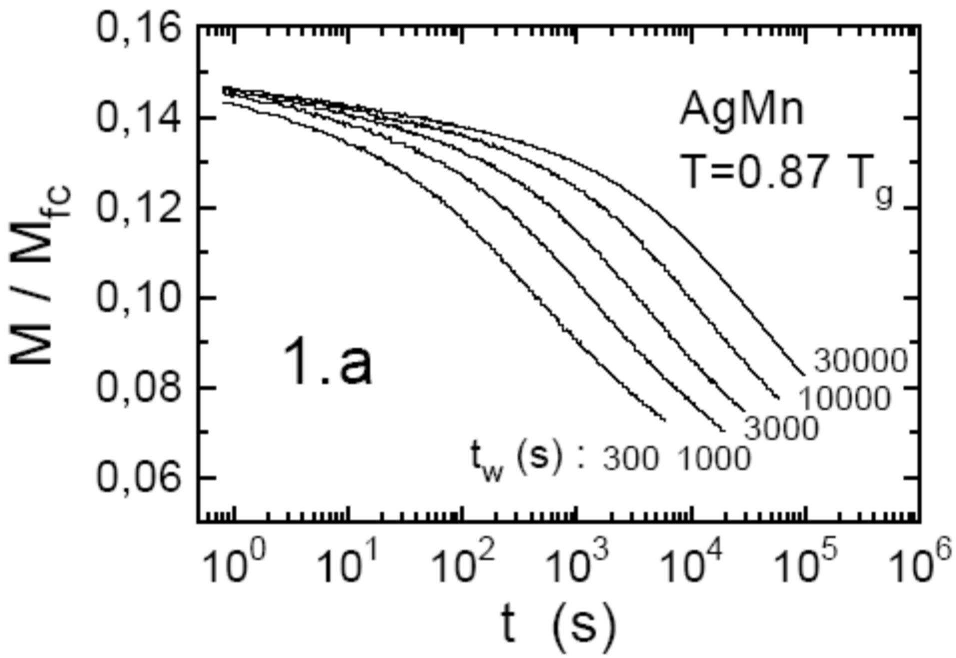
1. **Freezing of dynamics:** time scale slows down by many orders of magnitude

2. **Aging:** Response depends on a waiting time

3. **Coarsening**: Domains form, grow in time

(This work: only annealing, no shear)

II. Aging

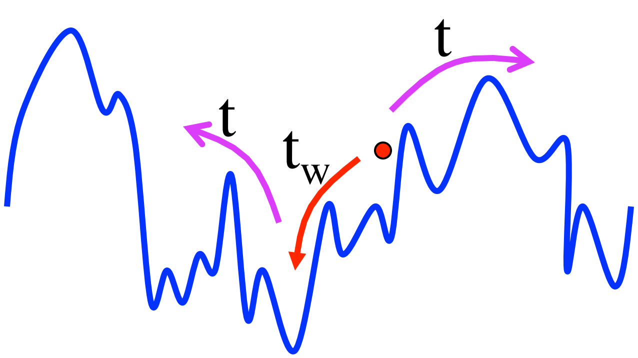


Spin Glass: Ag+2%Mn

1. Field cool
2. Wait for t_w
3. Measure relaxation

Response depends on the waiting time:

$$C(t, t_w) \neq C(t - t_w)$$



II. Aging

In mean field theory, $C(t, t_w)$ can assume scaling forms:

1. <u>Full/simple aging</u>: $C(t_w, t+t_w) = C_{eq}(t)\, C_{aging}(t/t_w)$

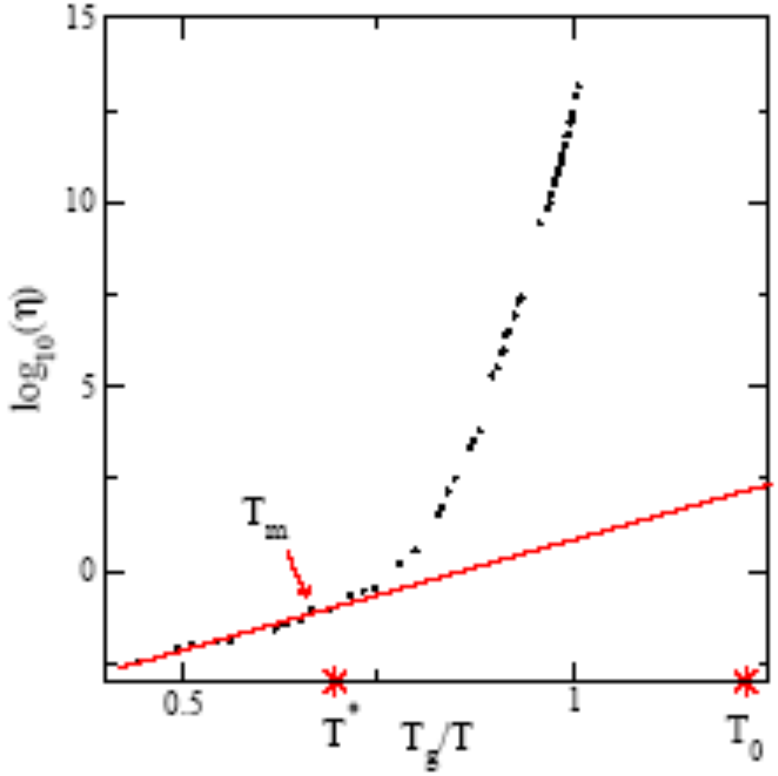
2. <u>Super/sub-aging</u>: $C(t_w, t+t_w) = C_{eq}(t)\, C_{aging}(t/t_w^{\mu})$

$\mu>1$ (superaging) and $\mu<1$ (subaging) have been observed experimentally and numerically

3. <u>Activated aging</u>: $C_{aging}(h(t+t_w)/\, h(t)) = C_{aging}(\ln(t+t_w)/\, \ln(t))$

Worked very well for the 3D Heisenberg spin glass.

II. Freezing of Dynamics



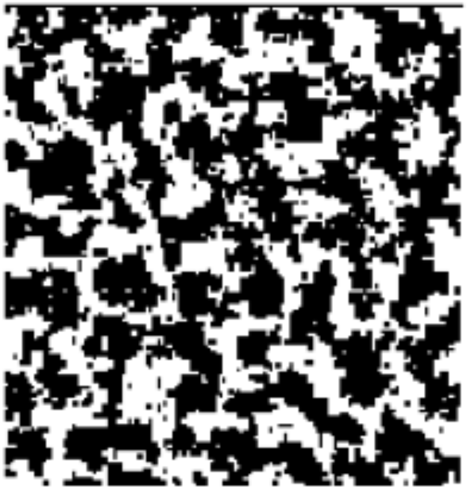
Super Arrhenius law for viscosity:

1. T_G finite, τ~exp[1/(T-TG)]
Vogel-Fulcher

2. T_G zero: avoided criticality
Kivelson

In practice: hard to distinguish, τ becomes immeasurably large at finite T

II. Coarsening



$t=10^3$ MC steps

$t=10^5$ MC steps

3D ordered Ising model,
Anneal to T<Tc

1. **Domains form**
2. **Domains grow**

II. Coarsening: Egyptian vases

Domains with increasing sizes
form on a time scale of thousands of years

II. Coarsening: Ordered, Disordered Systems

1. Ordered systems: $L \sim t^{1/z}$, $z=2$

Theory: infinite D, mode coupling: hard to identify length
Recently, Landau theory: growing length scales studied
(Chamon et al, 2002)
Results can depend on dynamics: Kawasaki: z=3

2. Disordered systems: $L \sim (T \log t)^{1/\psi}$ "z=0"

Energy barriers scale as $E \sim L^{\psi}$
Time to overcome barriers by activated dynamics:

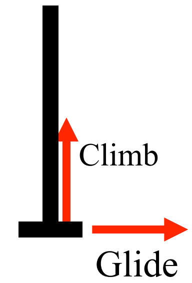
$$t \sim \exp(E/kT) \sim \exp(L^{\psi}/kT)$$

Non-frustrated randomness (RFIM): Yes
Frustrated randomness (EA): less clear

III. Simulations: Aristotelian Dynamics

Kroner continuum formulation:

$$D\Delta^2\chi = (b_x\partial_y - b_y\partial_x)\rho, \quad \sigma_{ij} = \frac{\partial^2\chi}{\partial x_i \partial x_j}, \quad \vec{f}_{PK} = \overleftrightarrow{\sigma}\vec{b}\hat{z}$$



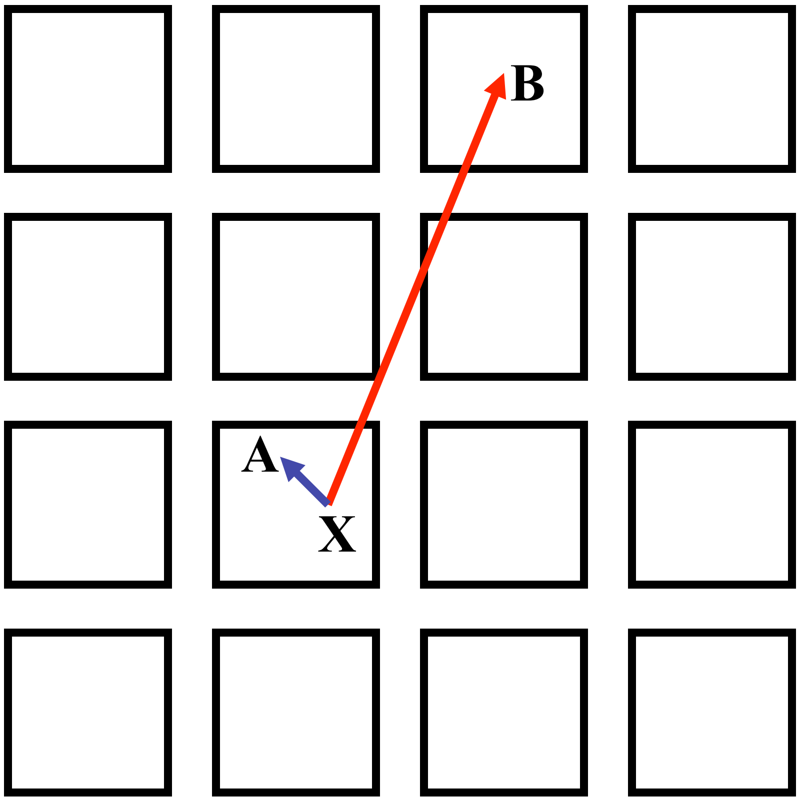
$$\vec{v} = B_g \vec{n}_g \tau_g^{PK}(r) + B_c \vec{n}_c \tau_c^{PK}(r)$$

1. **Overdamped (Aristotelian) dynamics**
2. **$\tau_{g/c}$ is the glide/climb component of the stress-related Peach-Kohler force**
3. **Dislocation interaction is in-plane dipole-dipole type ("vector Coulomb gas")**
4. **No external disorder**

Features

1. **Glide and climb (mobility: B_g, B_c)**
2. **Annihilation**
3. **Thermal force**
4. **Advanced acceleration technique**
5. **Rotation**

III. Fast Fourier Multipole Expansion



1. Divide simulation space into boxes:
   40,000 dislocations, 60,000 boxes
2. Calculate intra box interactions
   AX in real space
3. Calculate interbox interactions BX
   by calculating stress by Fast
   Fourier transformation
4. Move dislocations by eq. of motion
5. Repeat from 2

III. Simulation Features

Polarized - Non-polarized

1 glide axis - 3 glide axes

Climb - No Climb

Annihilation - No annihilation

$T=0$ - $T>0$

Rotation - No rotation

IV. Simulation Results: No Climb

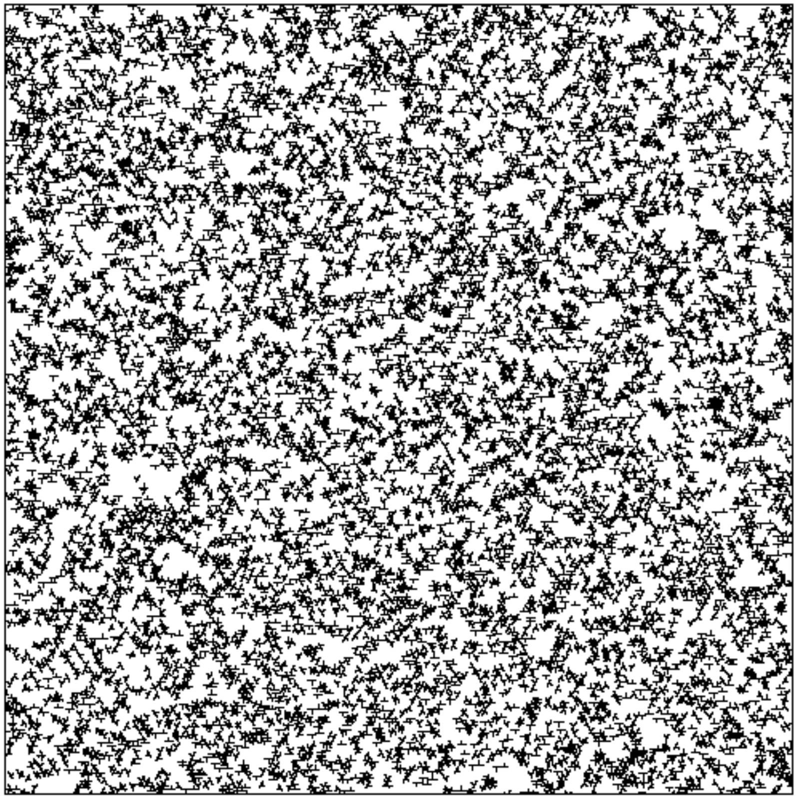
3 Glide axes

Non-polarized

Glide only, no Climb

No annihilation

Limited structure formation

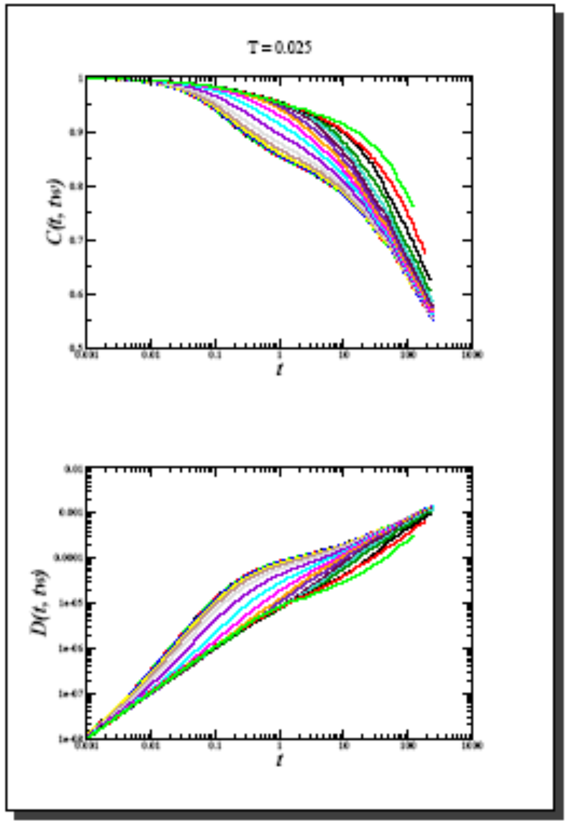


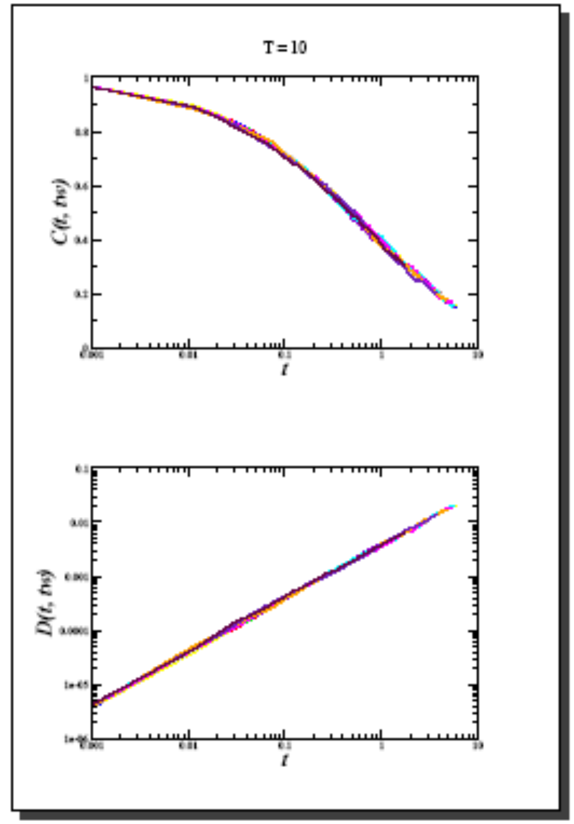
IV. No Climb: Aging

T=0.025 T=10

Self-overlap

Effective diffusion



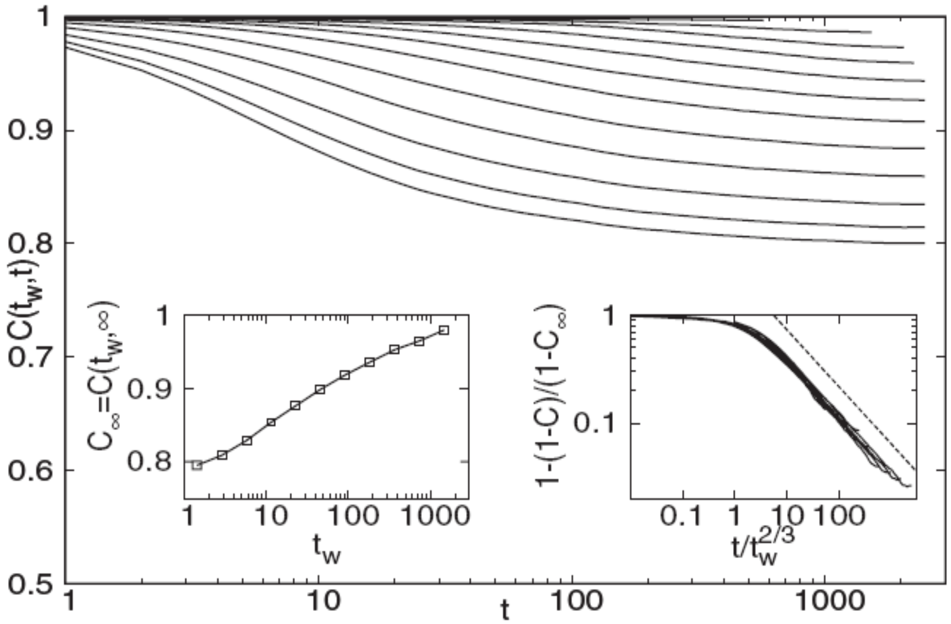


$$C(t,t_w) = \frac{1}{N_d}\sum_{i=1}^{N_d} \exp[-const|\vec{r}_i(t+t_w)-\vec{r}_i(t_w)|] \qquad D(t,t_w) = \frac{1}{N_d}\sum_{i=1}^{N_d} |\vec{r}_i(t+t_w)-\vec{r}_i(t_w)|^2$$

At low temperatures system falls out of equilibrium

Measured quantities start depending on waiting time: Aging

IV. No Climb: (Near) Textbook Aging



$$C(t_w, t) = \frac{1}{N_d}\sum_{i=1}^{N_d} \exp[-|\mathbf{r}_i(t+t_w) - \mathbf{r}_i(t_w)|/r_0]$$

$C(t,t_w) = C_{eq}(t)\, C(t/t_w^{\mu})$

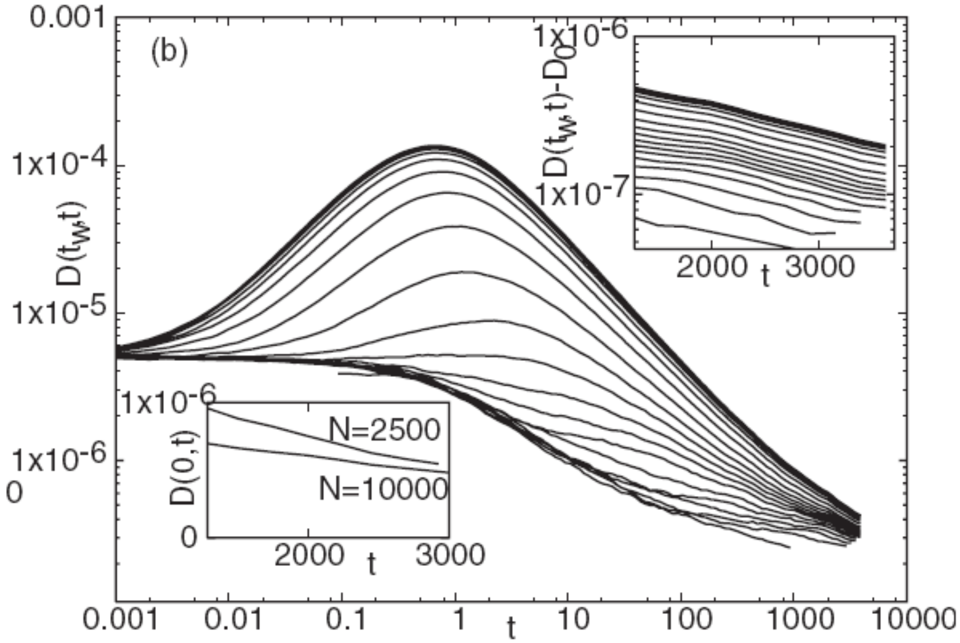
$C_{eq}(t) \sim t^{-\beta}$

μ=0.66, β=0.54

Analogous to spin glasses, since the location of the axes is a quenched randomness

μ is close to β

IV. No Climb: Freezing



$$D(t_w, t) = \frac{1}{N_d t} \sum_{i=1}^{N_d} |\mathbf{r}_i(t + t_w) - \mathbf{r}_i(t_w)|^2,$$

$D(t,t_w) \sim D(t_w)\, t^{-\gamma}$ T>0

$\gamma = 0.8$

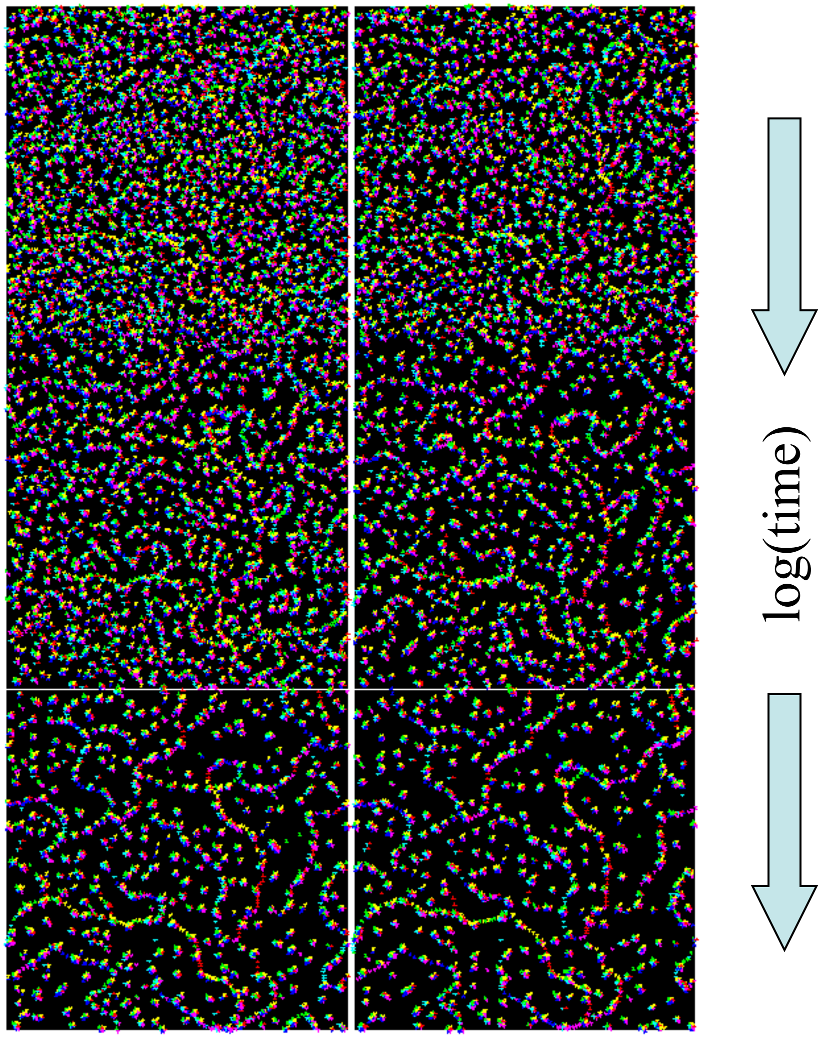
Diffusion constant goes to 0:

Freezing of dynamics

Aging and Freezing are evidence for:

Dislocation Glass

V. Climb+Annihilation: Wall/Domain Formation



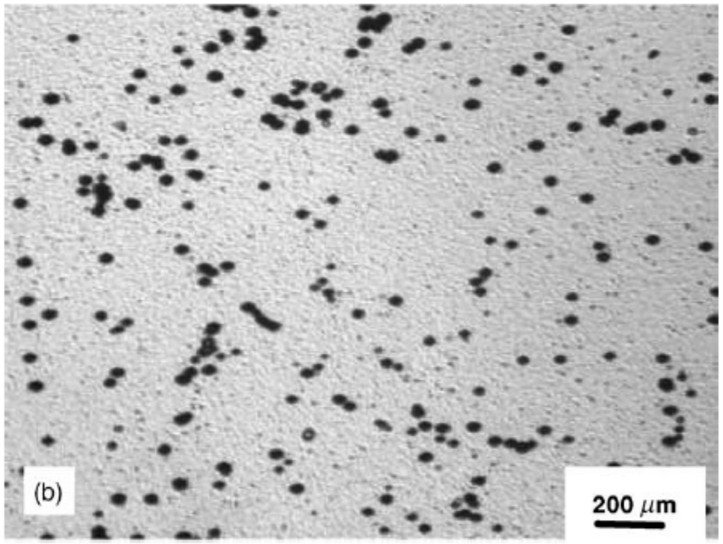
B_c/B_g=0.1

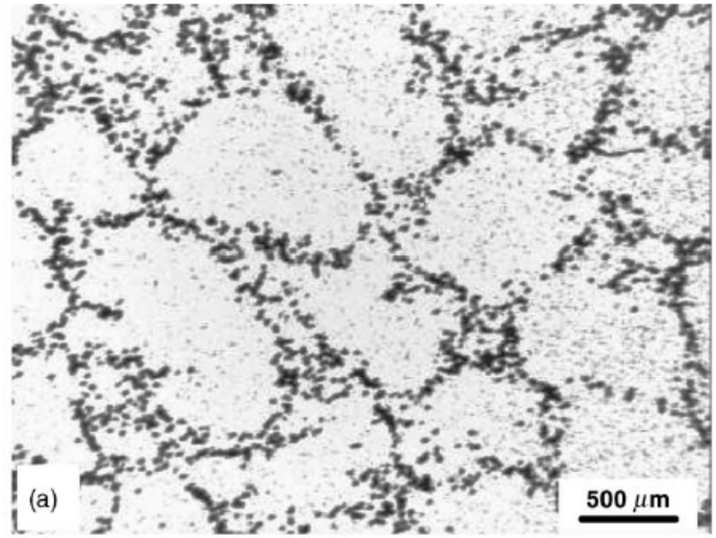
Glide, 3 slip axes, non-polarized: add climb, annihilation

- **Glide only:**
  10% of dislocations form walls, 90% remains in dipoles, which cannot annihilate
- **Glide+climb, annihilation:**
  Dislocations outside walls can annihilate, only walls remain

Domain formation induced by climb

V. Climb: Experiment: Climb Induces Domain Structures in GaAs



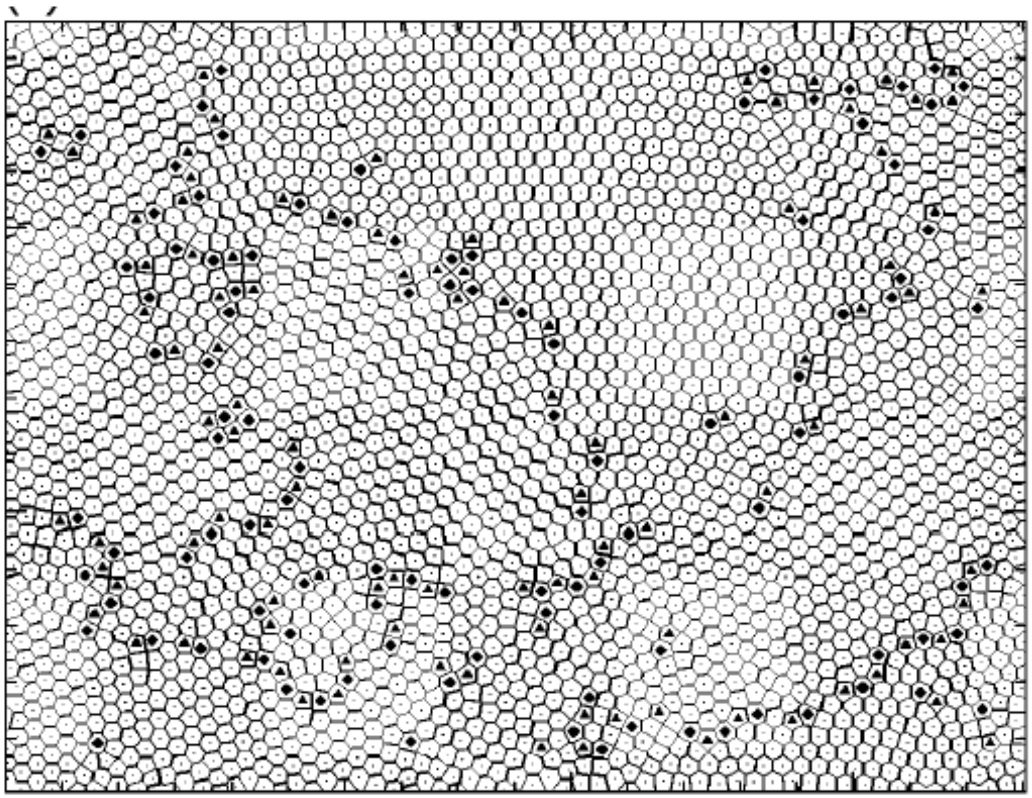


Climb

Rudolph et al. (2005)

Materials Science and Engineering A 400–401 (2005) 170–174

V. Climb: Experiment: Domain Formation in Dusty Plasmas



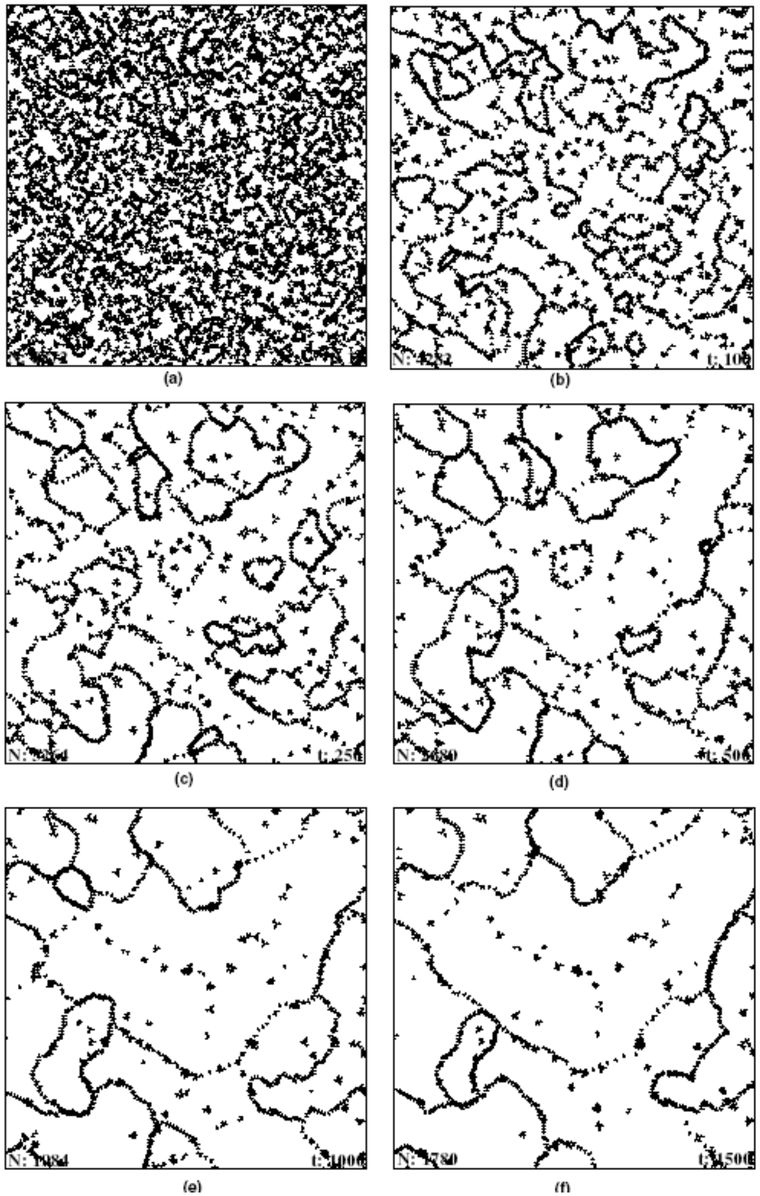
Quinn, Goree, 2001

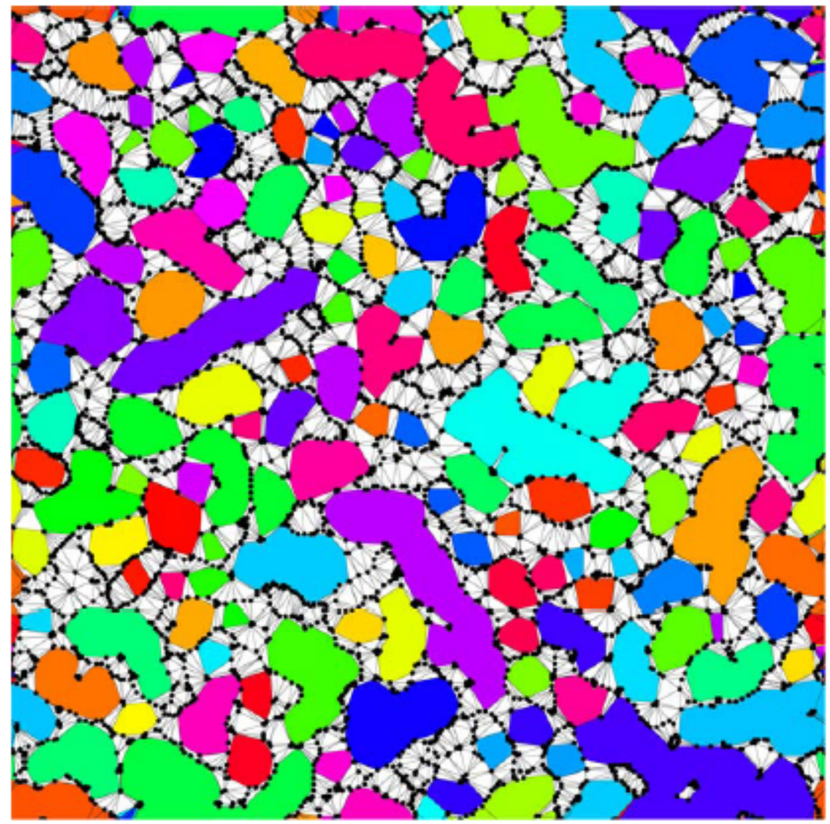
Charged particles settle

Climb is present

Domain formation

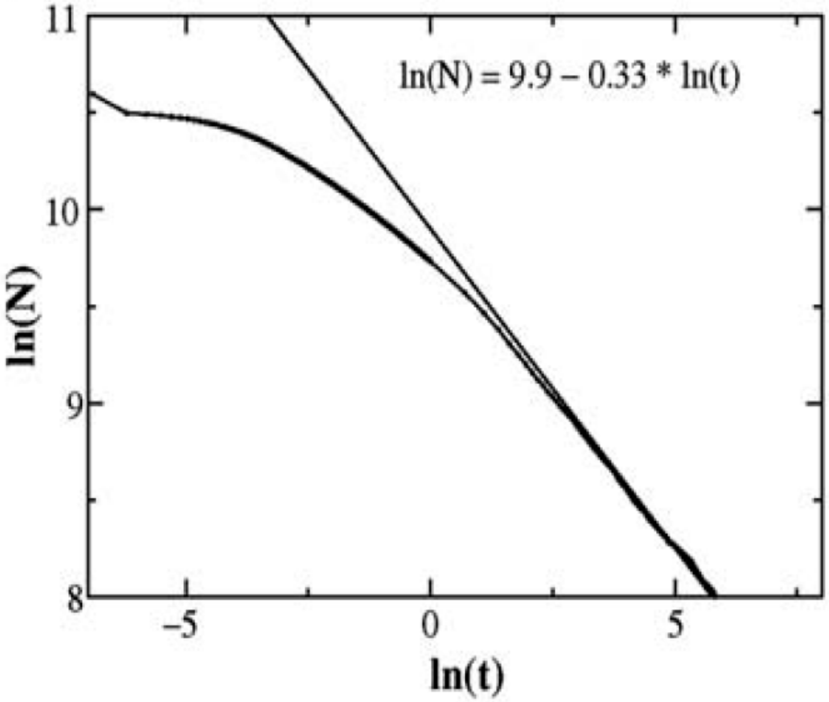
V. Climb: Coarsening

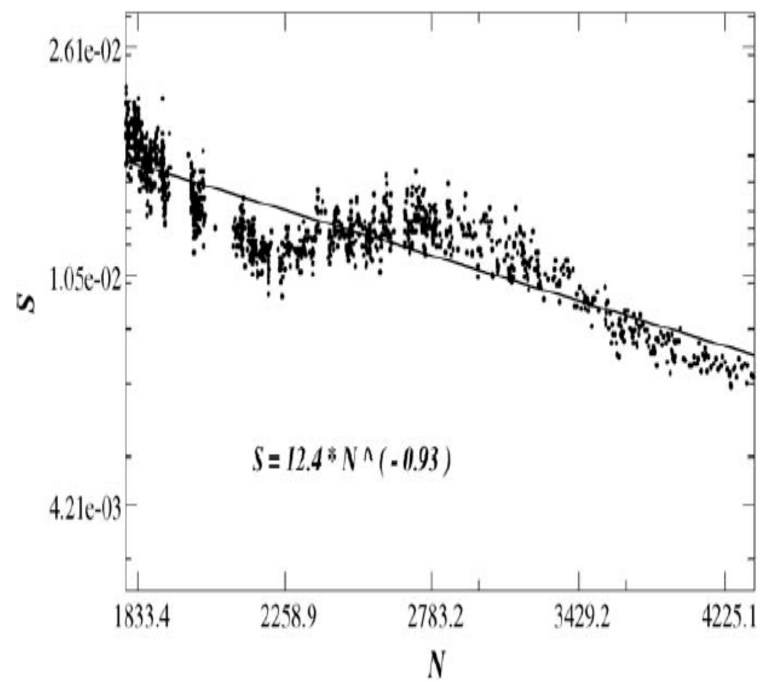




Domain size grows with time
Number of dislocations decreases

V. Climb: Coarsening: z, Holt relation





Number of dislocations: $N \sim t^{-0.33}$
Ave. distance between dislocations $L \sim 1/N^{1/2}$

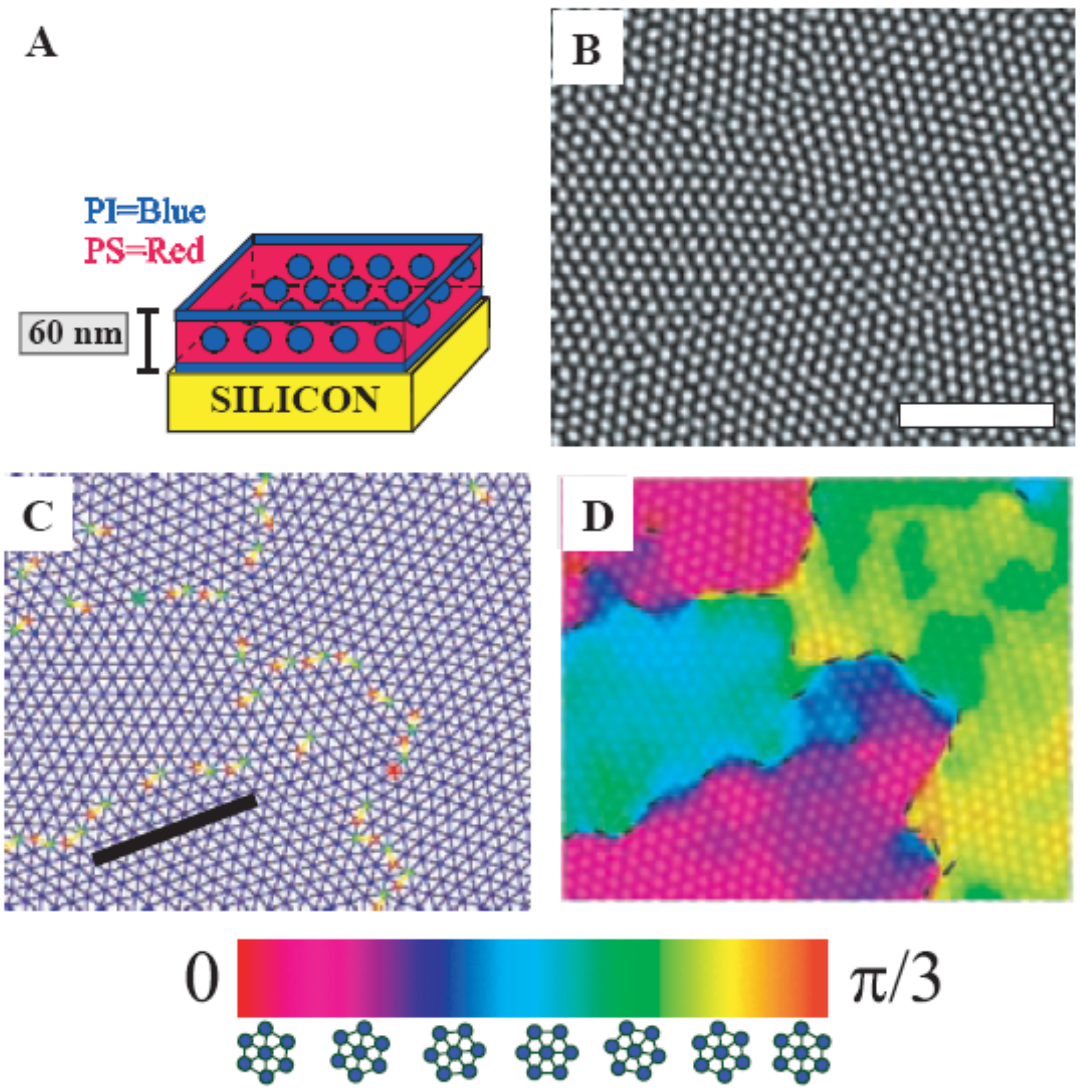
$L \sim t^{1/z}$

$1/z \sim 0.17$

Holt relation: cell area S
$S \sim N^{-1}$

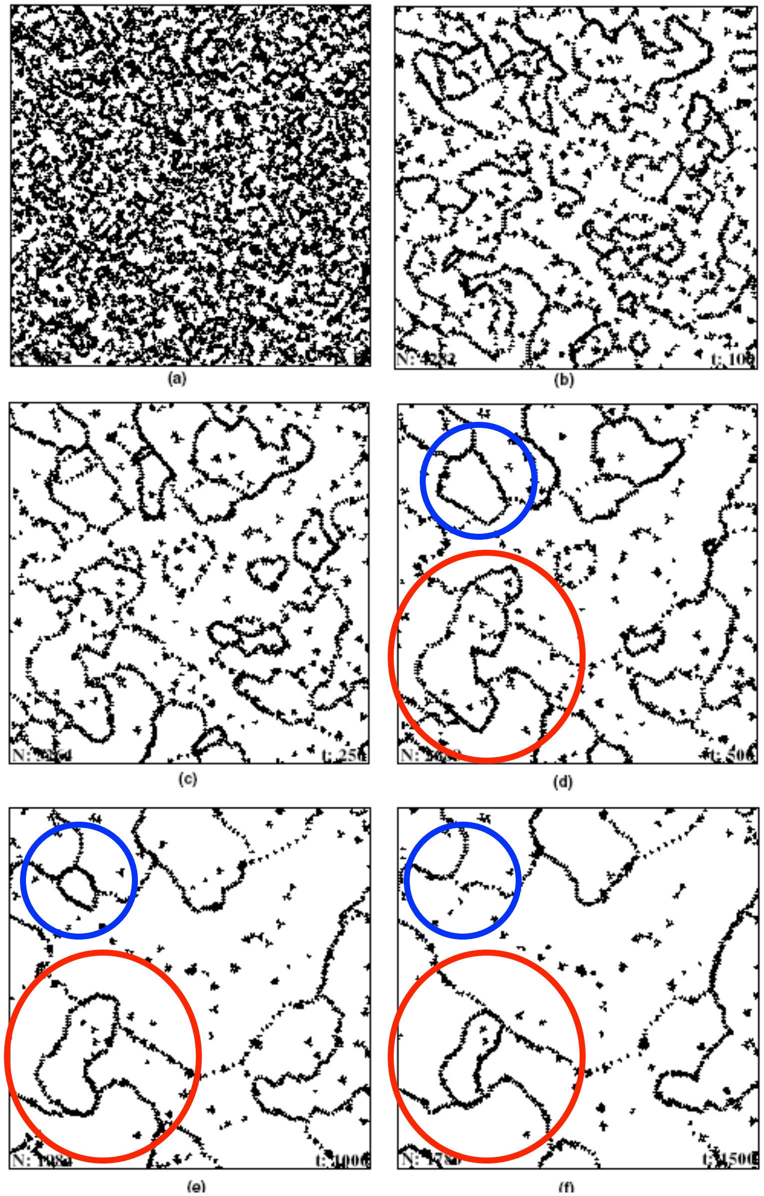
We measured S independently by a domain identifying search

V. Coarsening in Di-block copolymers



Chaikin, Huse, 2004
previous talk

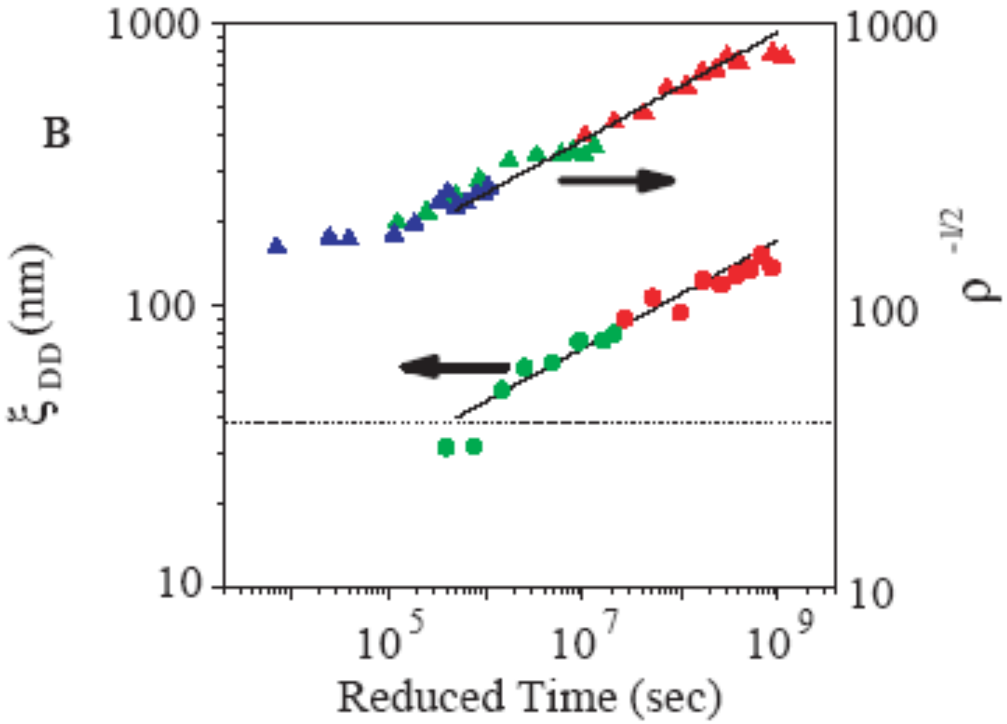
V. Coarsening by Domain Absorption



Coarsening happens by smaller domains getting absorbed at the boundaries of bigger domains.

Connection to polymers

V. Coarsening Exponent: 1/z=0.19



Remarkable agreement with our result of 1/z=0.17

V. Summary of Part I.

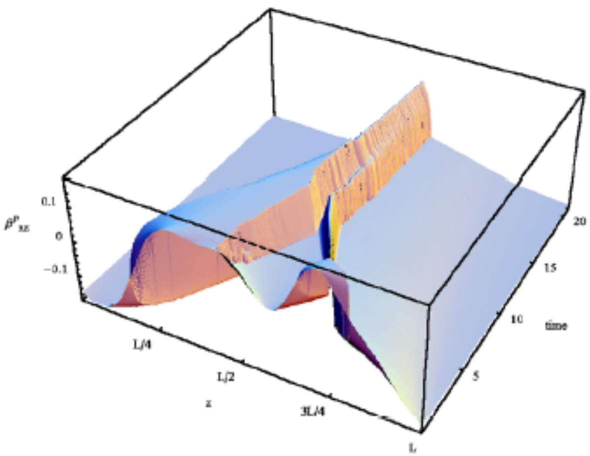
1. **Glide only model**
   - Aging: sub-aging scaling with waiting time
   - Freezing: effective diffusion constant goes to zero
   - Evidence for Dislocation Glass
   - Limited domain formation

2. **Glide + climb model**
   - Domain formation
   - Coarsening with exponent related to experiment

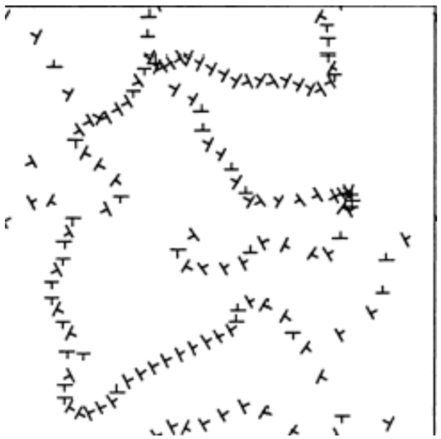
Proceed to understanding domain wall formation in detail

VI. Understanding Wall Formation

Sethna-Linkumnerd (2006)

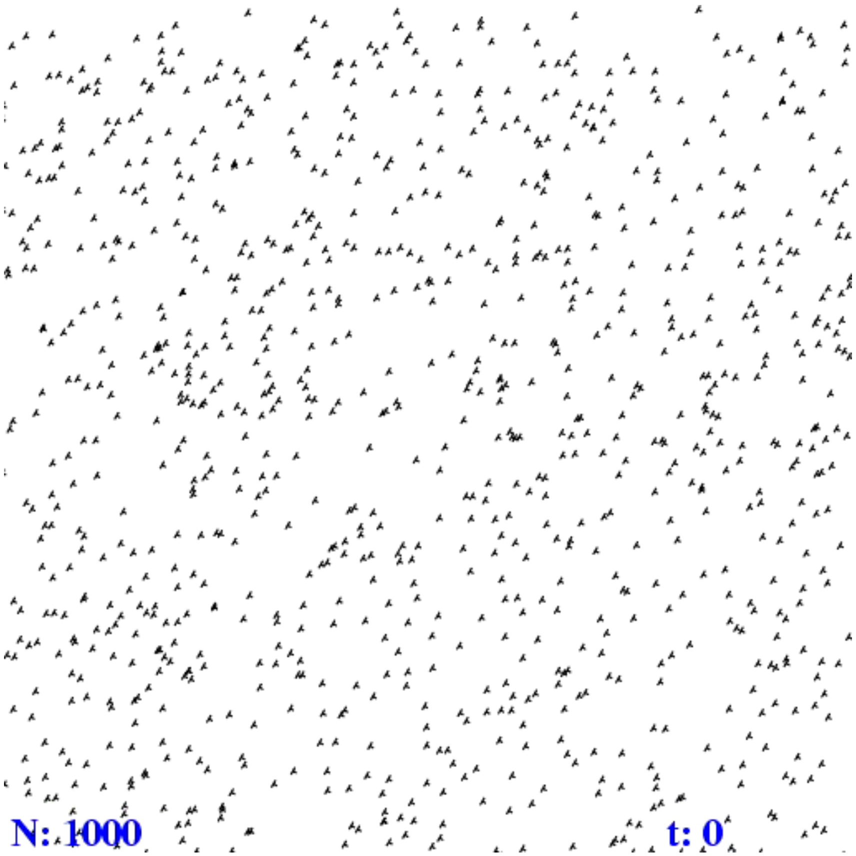


Argaman (2001)

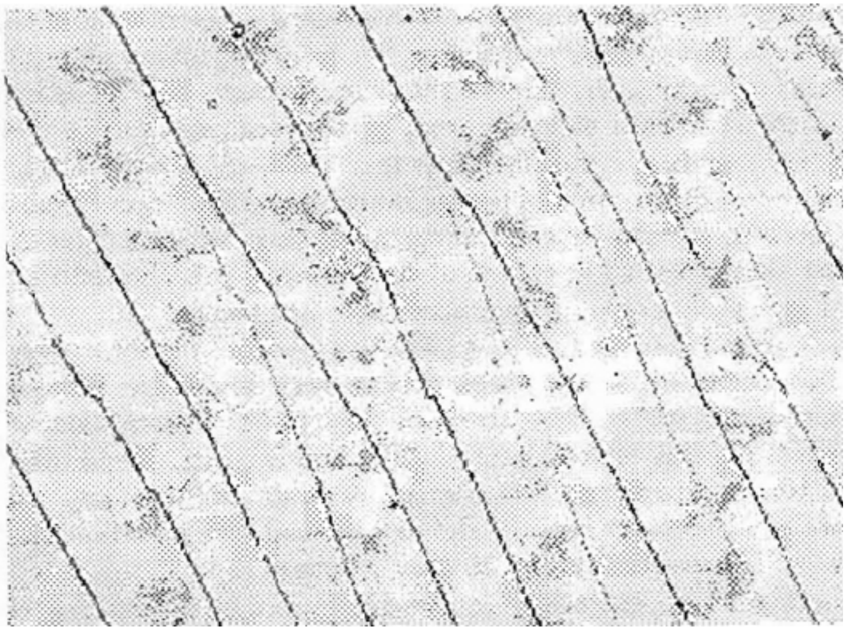


also, Barts-Carlson (1995)

VI. Glide only, Polarized: Wall Formation

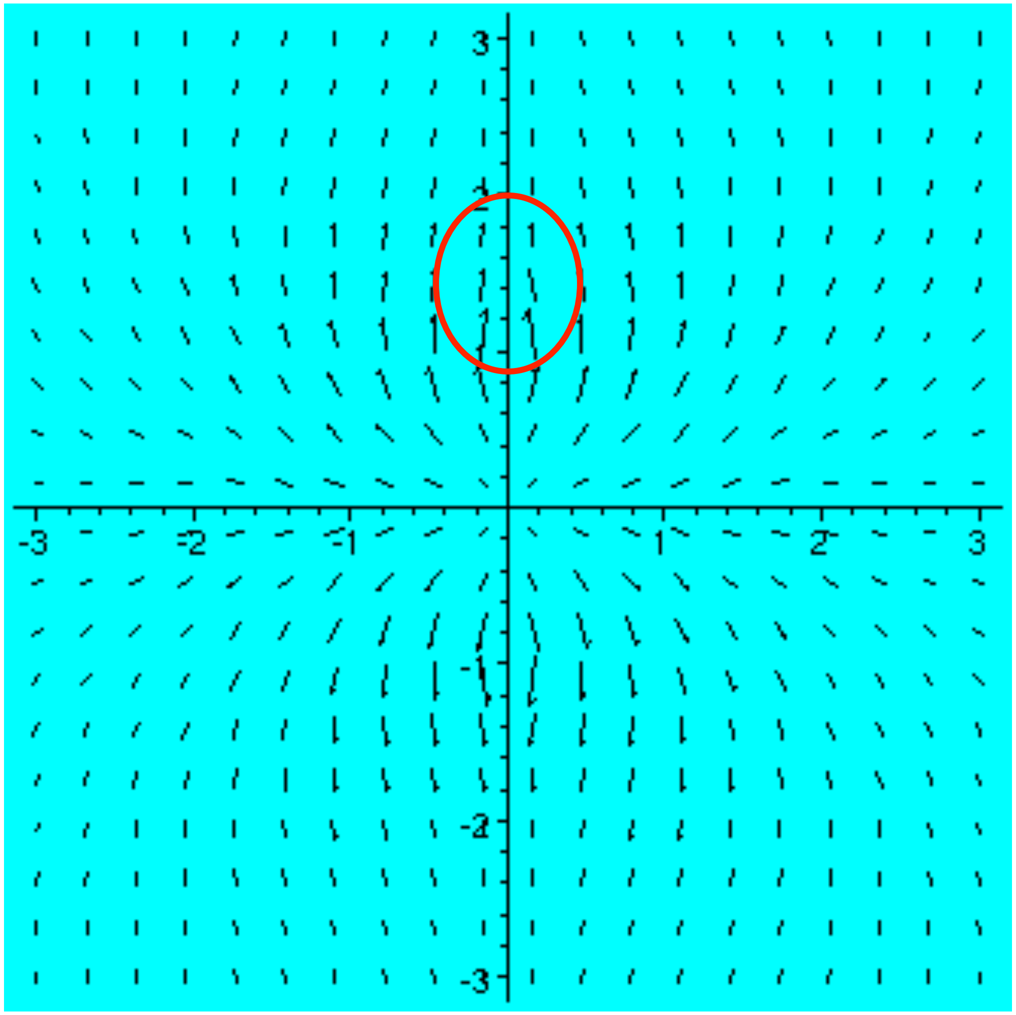


- Dislocations glide along 1 axis
- Walls are energetically favorable…



Fe-Si, Hibbard-Dunn T=925C

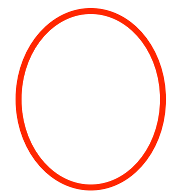
VI. Glide builds walls, climb destroys them?!?



Continuous wall: (0,-1) to (0,1)

Force on like dislocations:

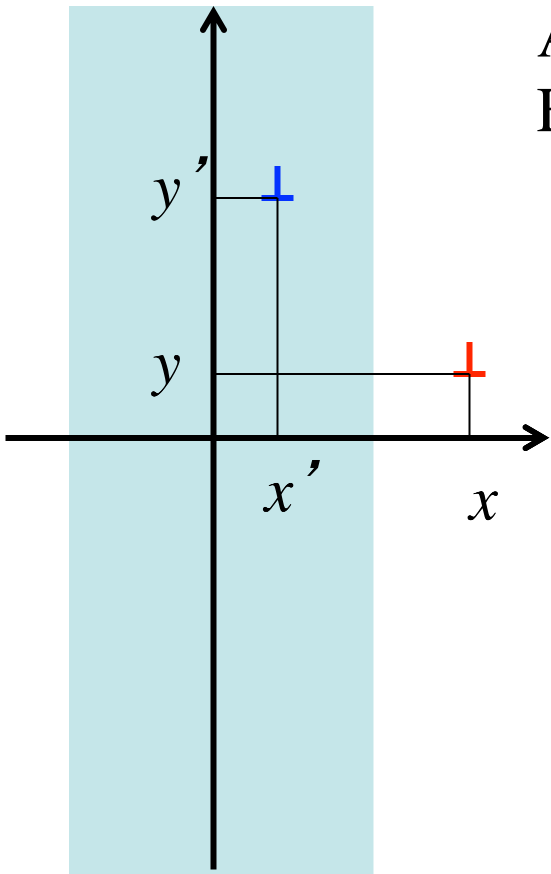
Glide only:
- repulsive on side
- attractive at ends only



Glide+climb:
- repulsive everywhere ?!?

VI. Glide: really no attraction from the side?

Self-consistent Potential Approximation (SPA)



All individual dislocations cannot be traced

Evolve the distribution of the dislocations $P_u(x)$

$$F_x(x) = \int_{-L}^{L} dy' \int dx' P_u(x') F(x - x', y - y')$$

$$\frac{dx}{dt} = BF_x(x)$$

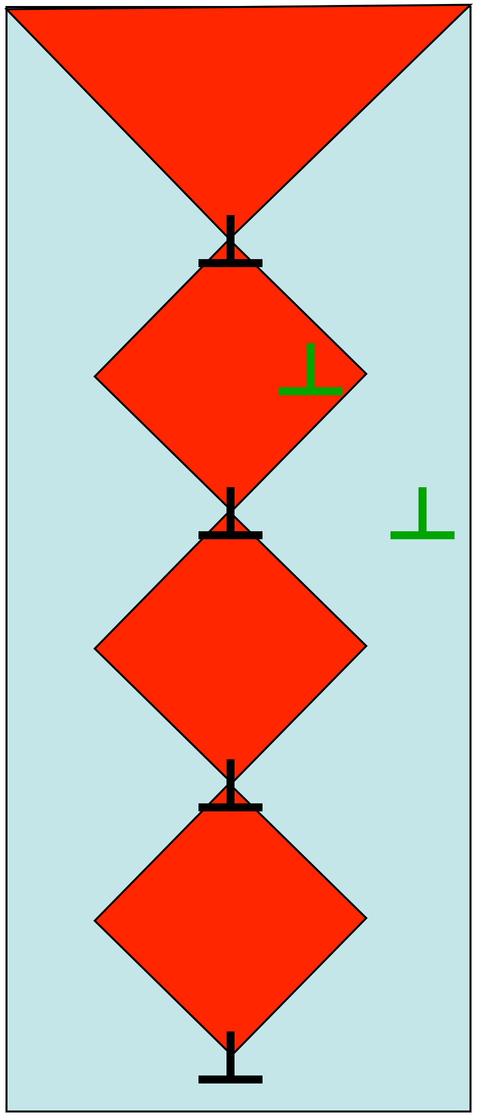
$$u(t) = \int dx \, P_u(x) x$$

Self-consistency

No attraction from side.

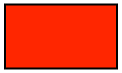
But: we assumed continuum limit!

VI. Discreteness Essential for Wall formation



Force on like (green) DL close to wall:

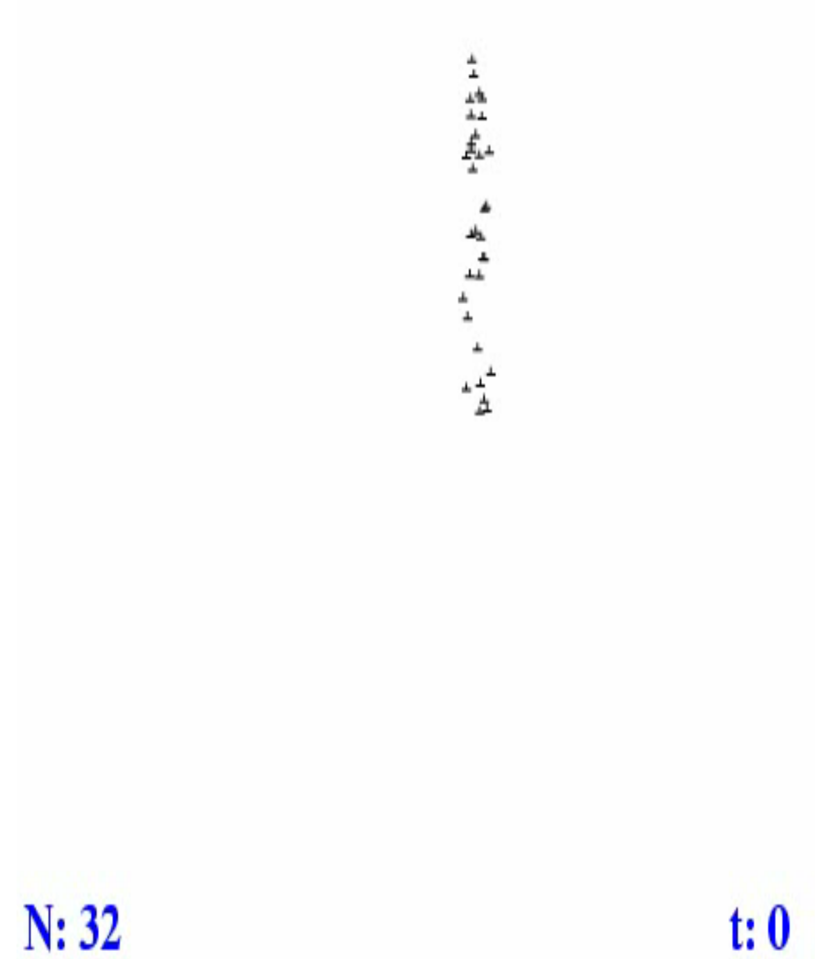
Repulsive: 

Attractive: 

Growth from the side:
only in the attractive diamonds,
generated by discreteness

Growth from the end:
attractive funnel at end

VI. Glide: Wall Formation: Simulation



1. The dislocations outside the attractive red diamonds of their neighbors fly out

2. Wall reassembles slowly, through
 - attractive side-diamonds
 - end-funnels

VI. Glide: Walls in Field Theory: Reverse Diffusion

$$D\Delta^2\chi = b\partial_y\rho$$

χ: Airy Potential

$$f = b\tau = b\partial_x\partial_y\chi$$

f: Peach-Kohler force

$$j = \rho v = \rho B f$$

$$j = \rho B b\partial_x\partial_y\chi + BT\partial_x\rho$$

Simplest extra term to capture discreteness

$$\partial_t\rho = ibB\rho_0 k_x^2 k_y \chi(k) + BTk_x^2\rho(k)$$

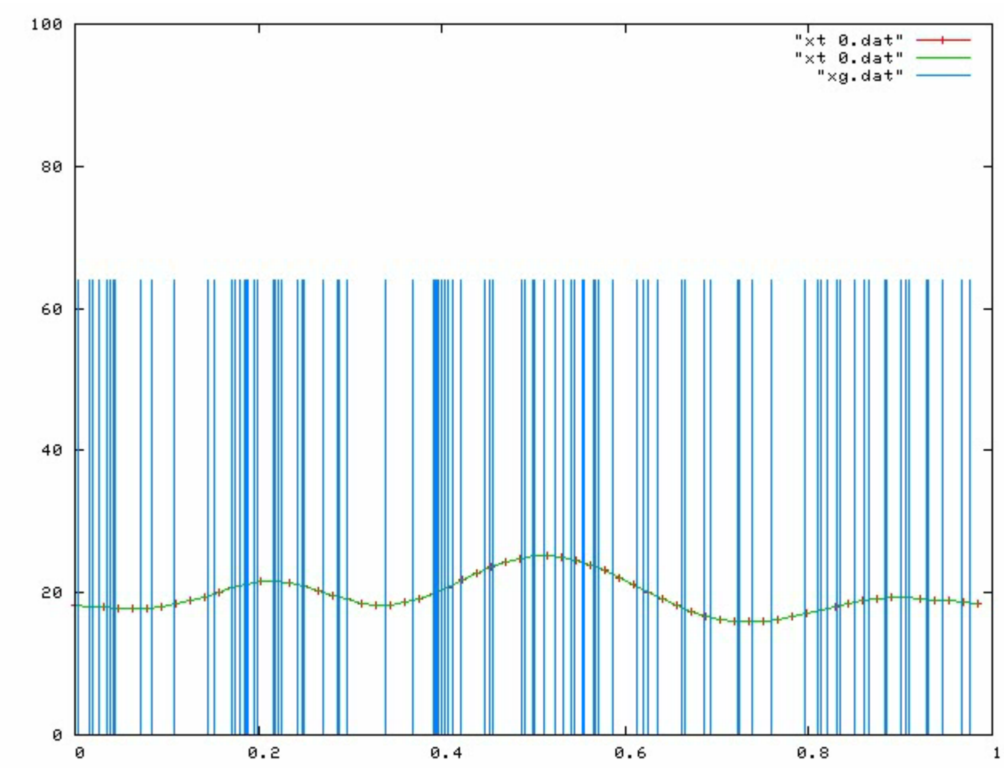
$$\partial_t\rho = [-Bb^2\rho_0\frac{k_x^2 k_y^2}{Dk^4} + TBk_x^2]\rho(k)$$

Without extra term: Fluctuations/walls do not grow

$$\partial_t\rho = BTk_x^2\rho(k) \qquad k_y = 0$$

Extra term and k_y=0: Unstable at every k_x, Larger k_x modes grow faster

VI. Glide: Reverse Diffusion: Simulation



$$\partial_t \rho = const. \times \partial^2 \rho / \partial x^2$$

Positive curvature (maxima):
always grow

Negative curvature (minima):
always decay

Walls indeed form!

Where the initial conditions had maxima

Length scale for fluctuations of initial condition is $\sim 1/\rho^{1/2}$

So distance between walls $d \sim 1/\rho^{1/2}$: Holt relation satisfied

VII. Glide+Climb: What Keeps Walls Together?

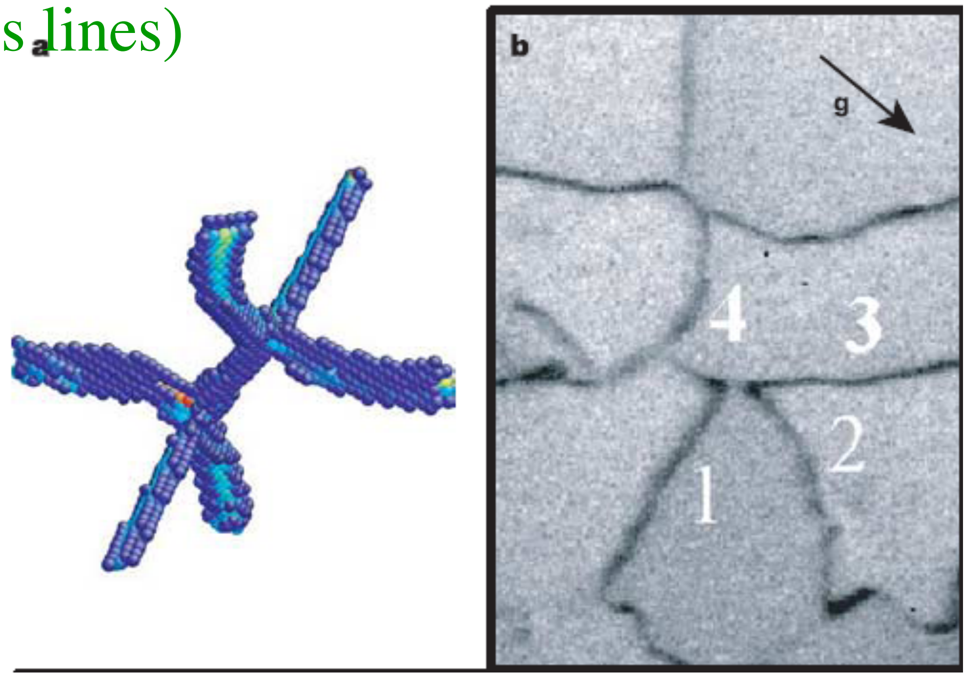
We saw in part I that climb is essential for wall formation.
Yet, climb seems to allow walls flying apart.
Why don't walls fly apart when climb is present?

3D: Junctions stabilize the patterns
(entangled/zipped dislocations lines)

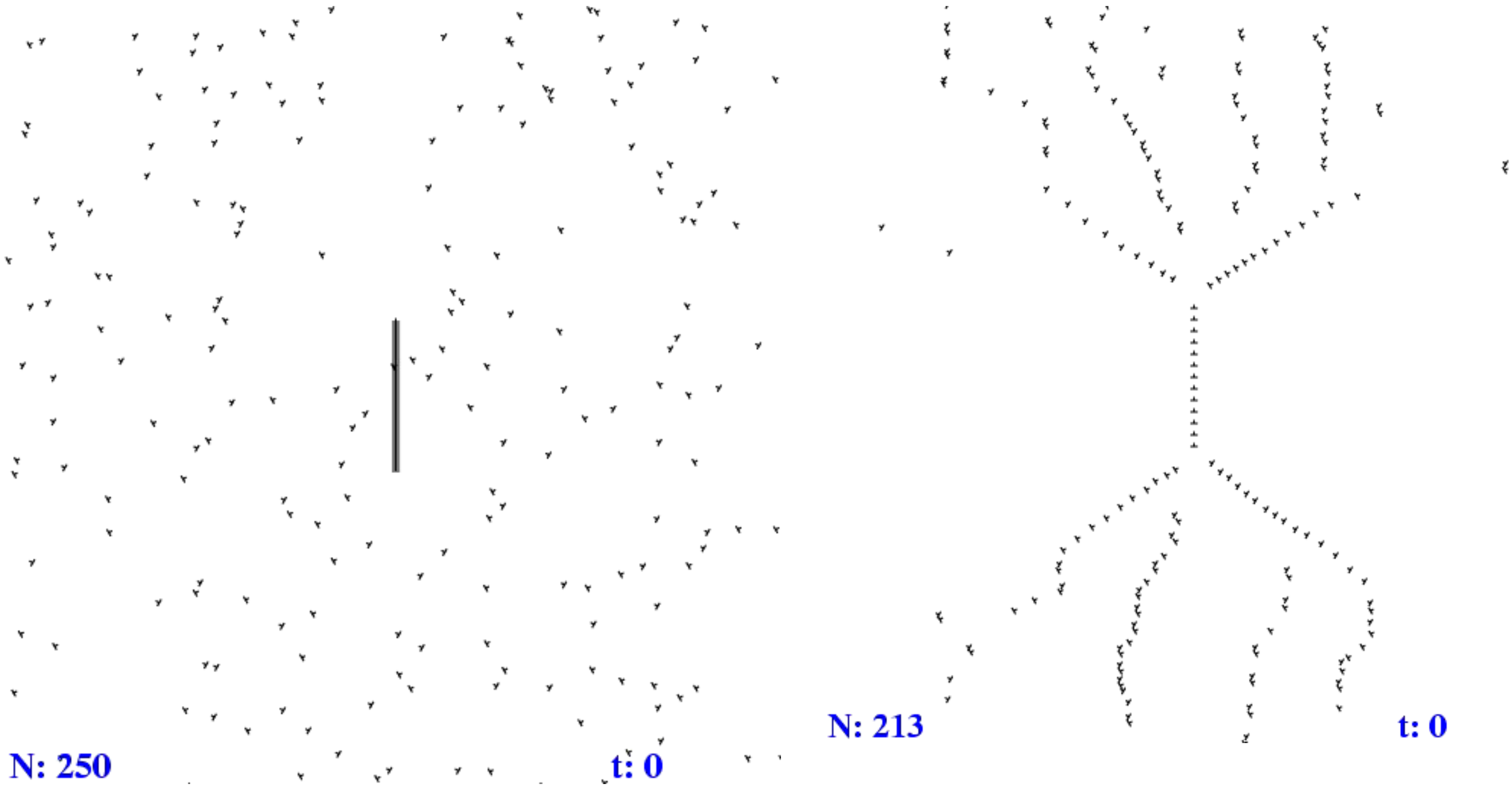
Bulatov (2006)

Kubin (next talk)

But: no junctions in 2D

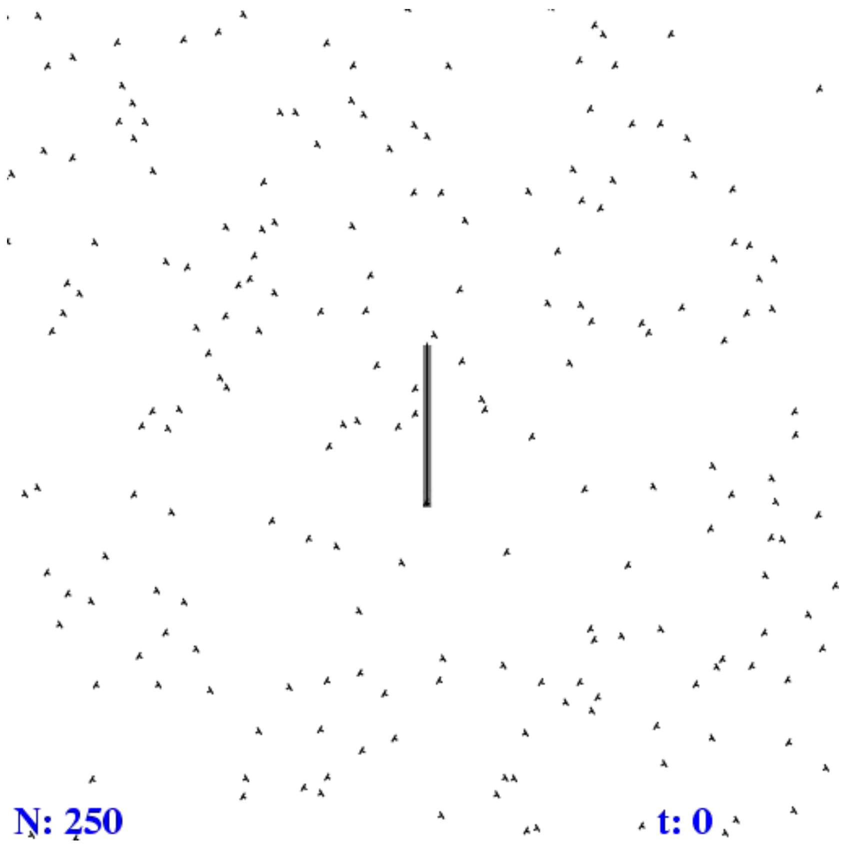


VII. Anchors Stabilize Against Climb



There are no junctions in 2D: what stabilizes structures?
Anchors stabilize domain walls effectively against climb

VII. Anchors Stabilize Against Climb



Anchors stabilize domain walls effectively against climb

VII. Ingredients of Wall Formation

- Glide only + Polarized:
  Wall forms by attracting dislocations in “near field” and at end

- Glide only + Neutral:
  Forces from opposite dislocations frustrate wall formation:
  10% in walls, 90% between

- Glide + Climb:
  Climb allows opposite dislocations to annihilate
  Only like dislocations in walls survive

- Anchors:
  Stabilize walls against flying apart by climb

Summary

Glide: Aging, Freezing (D_{eff}=0): Dislocation Glass

Glide+Climb: Domain formation – Expt.

Glide+Climb: Coarsening: z=0.17 – Expt.

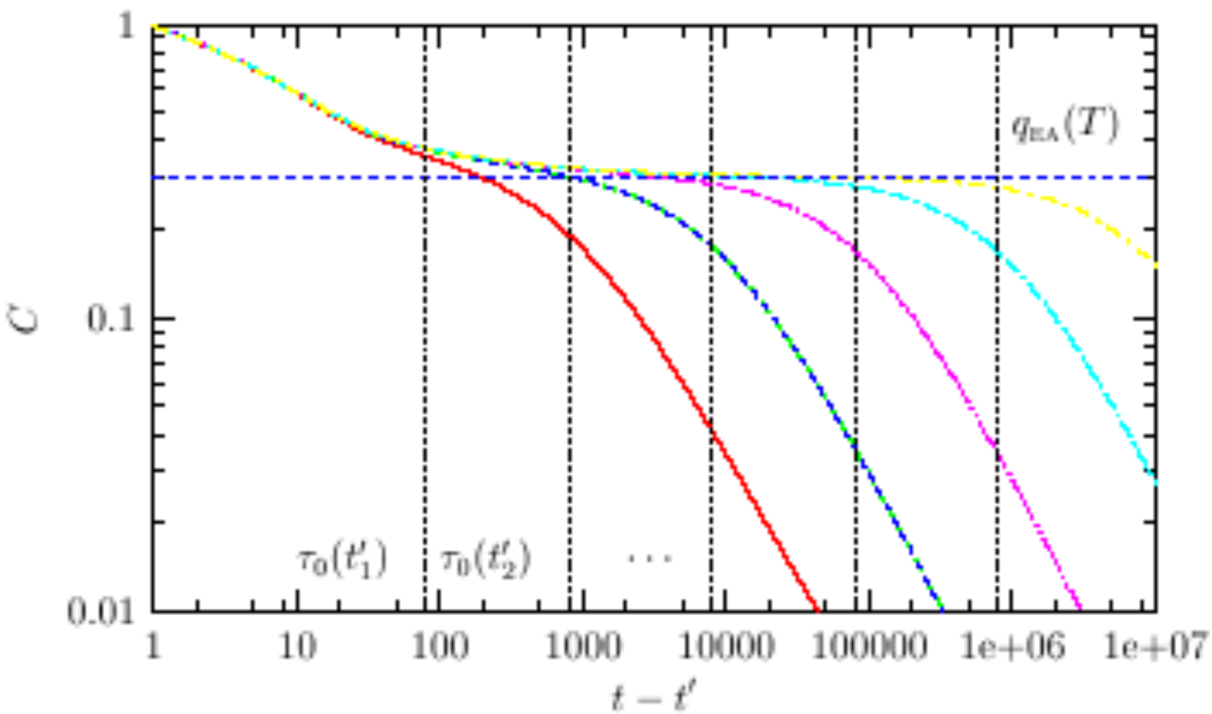
Walls/Glide: Attraction from near field – Sim’n

Walls/Glide: Reverse diffusion field th. – Sim’n

Walls/G+C: Anchors stabilize walls – Sim’n

Aging

Connection to equilibrium:
Correlation function C(t, t') exhibits a plateau
C(t, t') at plateau is the Edwards-Anderson (EA) order parameter



Increasing t_w, fixed T

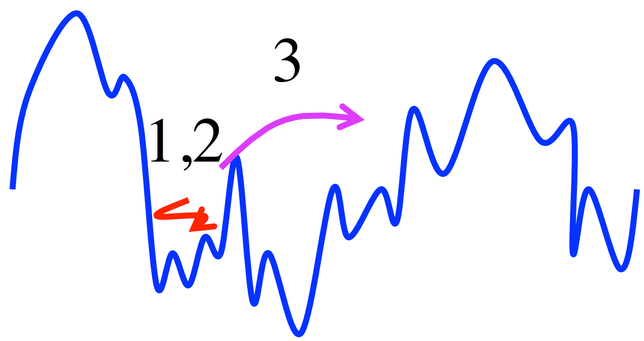
Aging

Stages:

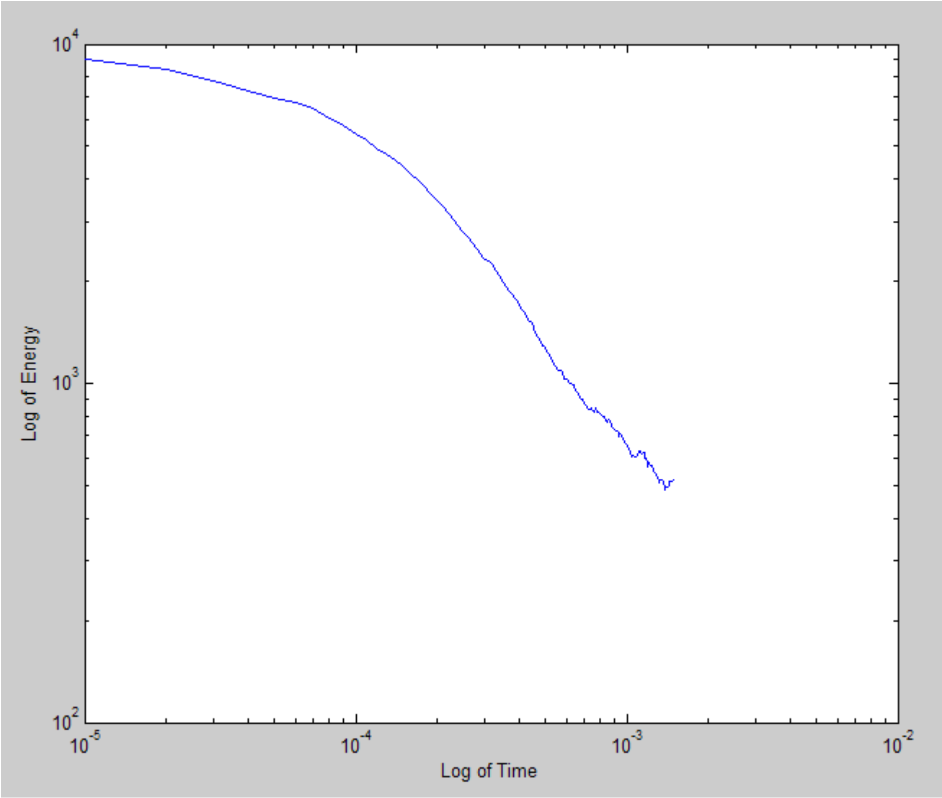
1. $t<t_w$: quick β relaxation: system expands from initial condition to explore boundaries of one well

2. $t \sim t_w$: plateau: system stuck within one well

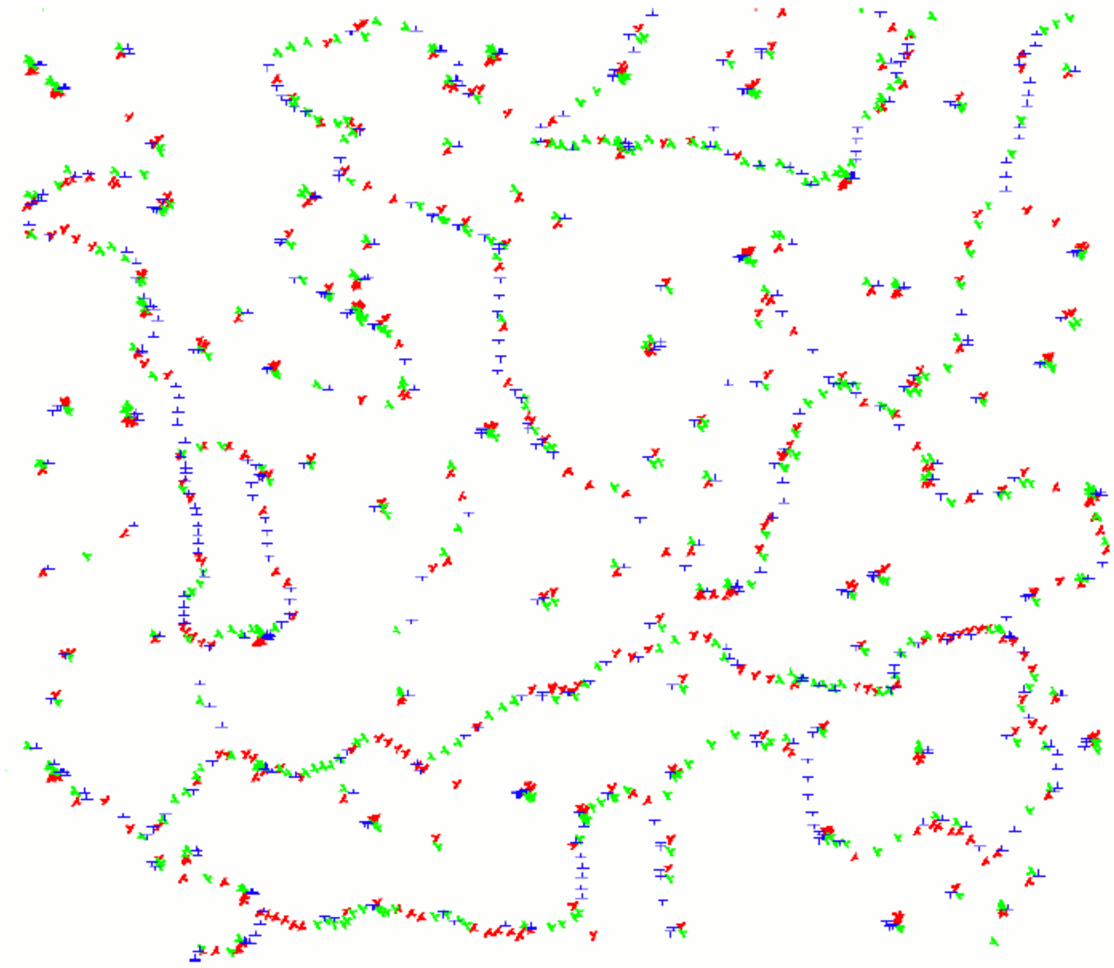
3. $t>t_w$: slow α relaxation: system escapes to other wells



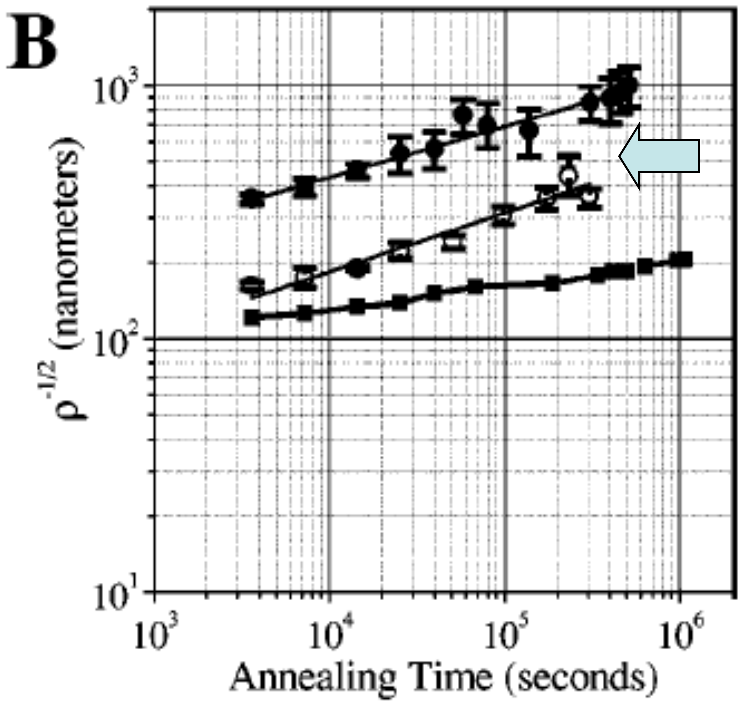
Glide only, 1 axis, Polarized: No Glassy Dynamics

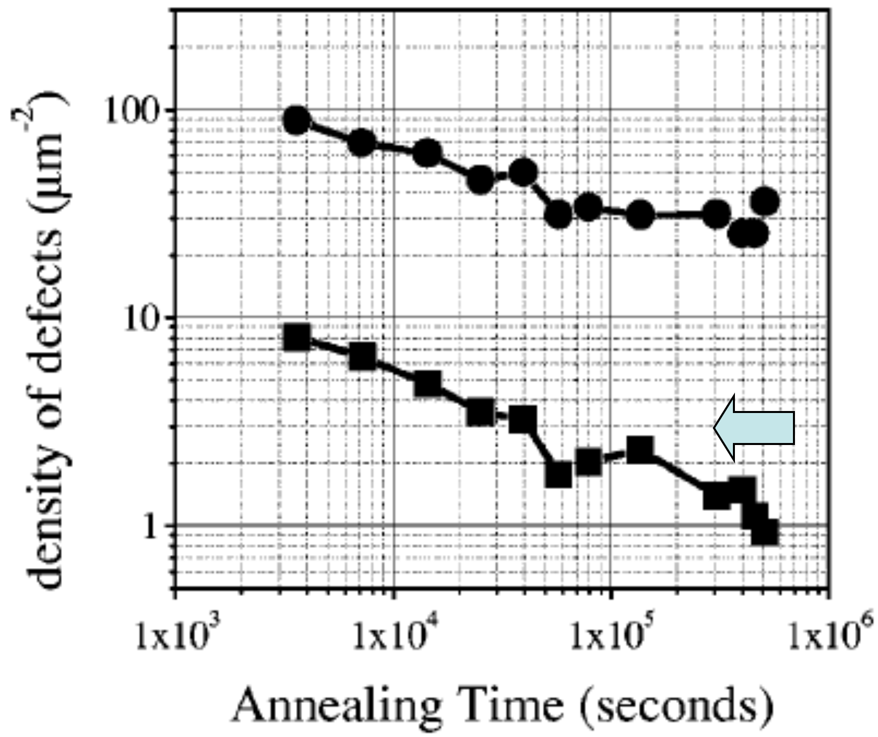


- No Aging
- $E(t) \sim t^{-1.4}$



The Coarsening Exponent is 1/4





$L \sim t^{1/4}$

Chaikin, Huse, 2002