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 (author’s image); (e) PbTe crystal grown by VB [33]; (f) SiC crystal grown by sublimation (courtesy of D. Siche from IKZ Berlin); (g) Cd_{0.99}Zn_{0.01}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].
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. **Full/simple aging**: $C(t_w, t+t_w) = C_{eq}(t) \ C_{\text{aging}}(t/t_w)$

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

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

3. **Activated aging**: $C_{\text{aging}}(h(t+t_w)/ h(t)) = C_{\text{aging}}(\ln(t+t_w)/ \ln(t))$

   Worked very well for the 3D Heisenberg spin glass.
II. Freezing of Dynamics

Super Arrhenius law for viscosity:

1. $T_G$ finite, $\tau \sim \exp[1/(T-T_G)]$
   
   Vogel-Fulcher

2. $T_G$ zero: avoided criticality
   
   Kivelson

In practice: hard to distinguish, $\tau$ becomes immeasurably large at finite $T$
II. Coarsening

3D ordered Ising model, Anneal to $T<T_c$

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: \( L \sim t^{1/z}, \quad z=2 \)

   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: \( L \sim (T \log t)^{1/\psi} \quad "z=0" \)

   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:

\[ D \Delta^2 \chi = (b_x \partial_y - b_y \partial_x) \rho, \quad \sigma_{ij} = \frac{\partial^2 \chi}{\partial x_i \partial x_j}, \quad f_{PK} = \tau \mathbf{b} \mathbf{z} \]

\[ \mathbf{\dot{v}} = B_g \mathbf{n}_g \mathbf{\tau}^{PK}_g (r) + B_c \mathbf{n}_c \mathbf{\tau}^{PK}_c (r) \]

Features

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

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
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

Self-overlap

Effective diffusion

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

At low temperatures system falls out of equilibrium
Measured quantities start depending on waiting time: Aging
IV. No Climb: (Near) Textbook Aging

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

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

$$\mu=0.66, \beta=0.54$$

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

$$\mu$$ is close to $$\beta$$

$$C(t_w, t) = \frac{1}{N_d} \sum_{i=1}^{N_d} \exp[-|r_i(t + t_w) - r_i(t_w)|/r_0]$$
IV. No Climb: Freezing

\[ D(t, t_w) \sim D(t_w) \; t^{-\gamma} \quad T>0 \]

\[ \gamma = 0.8 \]

Diffusion constant goes to 0:

Freezing of dynamics

Aging and Freezing are evidence for:

Dislocation Glass
V. Climb+Annihilation: Wall/Domain Formation

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

$B_c/B_g = 0.1$
V. Climb: Experiment: Climb Induces Domain Structures in GaAs

Rudolph et al. (2005)

V. Climb: Experiment: Domain Formation in Dusty Plasmas

Charged particles settle
Climb is present
Domain formation

Quinn, Goree, 2001
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 $L \sim 1/N^{1/2}$

$L \sim t^{1/z}$  
$1/z \approx 0.17$

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=925°C
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 $P_u(x)$

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

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

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

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

\[ D \Delta^2 \chi = b \partial_y \rho \]

\[ f = b \tau = b \partial_x \partial_y \chi \]

\[ j = \rho v = \rho B f \]

\[ j = \rho B b \partial_x \partial_y \chi + BT \partial_x \rho \]

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

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

\[ \partial_t \rho = BTk_x^2 \rho(k) \quad k_y = 0 \]

\( \chi \): Airy Potential

\( f \): Peach-Kohler force

Simplest extra term to capture discreteness

Without extra term:
Fluctuations/walls do not grow

Extra term and \( k_y = 0 \):
Unstable at every \( k_x \),
Larger \( k_x \) modes grow faster
VI. Glide: Reverse Diffusion: Simulation

\[ \partial_t \rho = \text{const.} \times \partial^2 \rho / \partial x^2 \]

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 ($D_{\text{eff}}=0$): 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 $\beta$ 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 $\alpha$ 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