Multiscale modelling of dislocation patterning

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to a high degree of disorder on various scales, stochas- μ ic methods are the needed to characterize and, possibly, possibly, possibly, possibly, possibly, possibly, μ tension, comparable micrographs from $\|f\|$ the literature have been considered (Cu f100g deformed to $\mathbb{E} \left\Vert \cdot \right\Vert$ $\left\Vert \cdot \right\Vert$ $\mathbb{E} \left\Vert \cdot \right\Vert$ and $\mathbb{E} \left\Vert \cdot \right\Vert$

• Multitude of observed dislocation patterns are interpreted in terms of an interpreted in the results are in the results are in the results are in the results are in the result by a hierarchy of mesoscopic scales (ranging from say α stochastic dislocation dynamical model of cell formation.

to describe properly defect microstructures which exhibit exhibit exhibit exhibit exhibit exhibit exhibit exhi

predict and control the structural features. Fractal analysis then provides a tool to account for multiscale behavior

- \bullet Fractal, periodic, etc.
- **Crucial impact on plastic properties Crucial impact on plastic properties**
- May lead to strain localization and failure of the material way lead to shall localization and

H Mughrabi, F Ackermann, K Herz, STP675, 1979 H Mughrabi, T Ungár, W Kienle, M Wilkens, Philos Mag, 1986 $\frac{1}{2}$ conguity in a currencture in a currencture conduction $\frac{1}{2}$

 $\frac{1}{2}$ $\frac{1}{2}$ in the stress $\frac{1}{2}$ in the actual stress in the ac ϵ and ϵ 37.3, ϵ 37.3, ϵ 37.3, ϵ 37.3, ϵ 37.3, ϵ 37.3, ϵ φ i π i ins parallel and normal to the total tot

 T the micrographs were digital binary maps were digital binary maps $\mathcal{L}_\mathbf{z}$

Dynamic modelling of PSBs

• Reaction-diffusion model:

$$
\partial_t \rho_i = D_i \partial_x^2 \rho_i + g(\rho_i) - \bar{P}\rho_i + c\rho_m \rho_i^2
$$

$$
\partial_t \rho_m = D_m \partial_x^2 \rho_m + \bar{P}\rho_i - c\rho_m \rho_i^2
$$

- $\hat{\rho}_{\rm m}, \rho_{\rm i}$: mobile and immobile dislocation densities
- $\bullet \ \ g(\rho)$: dipole generation/loss function
- \cdot \bar{P} : plastic strain rate
- \bullet c : pinning rate

D Walgraef, EC Aifantis, J Appl Phys, 1985 EC Aifantis, Int J Plast, 1987

(a) (b) $|ce||$ structures $\mathbf{H}[\mathbf{Y}]$ and $\mathbf{F}[\mathbf{Y}]$ and $\mathbf{F}[\mathbf{X}]$ and $\mathbf{F}[\mathbf{X}]$ and $\mathbf{F}[\mathbf{X}]$ and $\mathbf{F}[\mathbf{X}]$

- Mean-field 3D continuum dislocation dynamics model
- Enabling cross-slip leads to the formation of a cell structure

of the simulated cube and (b) distortion of a slice parallel to (001) plane. The linear \Box displacement associated with the average strain is suppressed and only the perturbation is suppressed and only the perturbation is suppressed and only the perturbation of \Box

displacement ∼**u** is displayed with a 200 times magnifcation.

S. Xia and A El-Azab, Mod Simul Mater Sci Eng, 2015 **Strain and Strain with cross slip activation** $\ddot{\theta}$

Continuum modelling of

- CDD model of Hochrainer and coworkers
- Neglecting elastic stress interactions and keepeng a Taylor-like friction stress leads to a cellular pattern

Objectives

- Multiscale modelling of dislocation patterning
	- Quantitative comparison of *discrete* and *continuum* models
	- Validation of the continuum model, e.g. back-stress
	- Systematic determination of the fitting parameters of the continuum model
	- Simplest case: 2D single slip

\blacksquare \rightarrow), \rightarrow , and \rightarrow 10, \rightarrow shear modulus and not the Poisson's ratio. The Poisson's ratio simulation cell L is set to unity and the simulation volume remains disordered tilt walls, which are periodic arrays of edge dislocations that a tilt and all and adjoining the second between two adjoining crystals. The development of low-misoriented tilt walls is suspected to be

 $\begin{vmatrix} \cdot & \text{With increasing strain} \end{vmatrix}$ dipolar walls form transient effects. We measure the average absolute value of the dis- $\begin{array}{|c|c|c|c|c|}\hline \quad & \quad & \mathbf{c}\end{array}$ i~1

is proportional to the stress, $\mathbb{F}_{\mathbb{F}_{q}}$, \mathbb{F}_{q} , \mathbb{F}_{q} , \mathbb{F}_{q} , \mathbb{F}_{q}

fixed throughout loading. In our normalized units, mb/2(12n)51 and g51. We initially relax the system without an applied external

As the randomly positioned dislocations relax under zero applied

. The external load on a dislocation and a dislocation

 \overline{a}

forms, P1250 and B5P11,22.

these are the 'strongest' | objects in 2D single slip current curve for superconductions \vert \blacksquare \blacksquare characterize the content and charge only

 $U\cup U$ unipolar walls composed of $U\cup X$ tive or positive or positive, as shown in Fig. 1(d). The interval behavior \mathcal{U}

a precursor for the eventual formation of \mathcal{A} in \mathcal{A} in

C Zhou, C Reichhardt, CJO Reichhardt, IJ Beyerlein, Sci Rep, 2015 Results and Discussion same in all panels. Red (blue): large negative (positive) stress. (a) The initial α

Results: evolution of density patterns

DDD configuration

Continuum total density ρ

Continuum GND density κ

Continuum models

• Evolution equations of dislocations

$$
\partial_t \rho_i + \nabla \boldsymbol{j}_i = f_{\text{reaction}}(\rho_i, \tau_{\text{ext}}, \dots)
$$

- \cdot ρ_i : some scalar dislocation density field
- \cdot \boldsymbol{j}_i : flux of the given density
- \bullet $f_{\rm reaction}$: multiplication, annihilation, cross-slip, etc.
- Question:
	- What scalar densities to use?
	- What is the reaction term?
	- How to compute the fluxes?

• In 2D single slip:

- SSD (ρ) and GND (κ) densities?
- No multiplication, no annihilation

 $\dot{5}\dot{5}\dot{5}$

Benchmark of continuum models

• Tensile test of a model composite material

294 *S. Ye!mov et al. / J. Mech. Phys. Solids 52 (2004) 279 – 300*

 \blacksquare

ρ*L²*

Continuum model of Groma

Equation of motion of individual dislocations

Coarse graining

Hierarchy of *N*-body densities

Assumption of short range correlations

Closed set of evolution equations for ρ and κ

I Groma, Phys Rev B, 1997

I Groma, M Zaiser, FF Csikor, Acta Mater, 2003

Evolution equations w/o correlations

$$
\partial_t \rho(\mathbf{r}, t) = -M_0 b \partial_x [\kappa \tau_{\text{mf}}]
$$

$$
\partial_t \kappa(\mathbf{r}, t) = -M_0 b \partial_x [\rho \tau_{\text{mf}}]
$$

- $\boldsymbol{\cdot} \ M_0$: dislocation mobility
- \bullet b : Burgers vector
- \bullet $\tau_{\rm mf}$: mean-field stress
	- External load & long-range stresses generated by the GNDs

$$
\tau_{\rm mf}(\bm{r},t)=\tau_{\rm ext}+\int \kappa(\bm{r}-\bm{r}')\tau_{\rm ind}(\bm{r}'){\rm d}^2r'
$$

- Measurable quantity: the average local stress around a dislocation
- Plastic strain: $\partial_t \kappa(\bm{r},t) = -(1/b) \partial_x \dot{\gamma}(\bm{r},t)$

Evolution equations with correlations

$$
\partial_t \rho(\mathbf{r}, t) = -M_0 b \partial_x [\kappa \tau_{\rm mf} + \kappa \tau_{\rm b} + \rho \tau_{\rm d}]
$$

$$
\partial_t \kappa(\mathbf{r}, t) = -M_0 b \partial_x \left[\rho \tau_{\rm mf} + \rho \tau_{\rm b} - \rho \left(1 - \frac{\kappa^2}{\rho^2} \right) \tau_{\rm f} + \kappa \tau_{\rm d} \right]
$$

• Back-stress:
$$
\tau_{\rm b}(\boldsymbol{r},t) = -Gb \frac{D}{\rho} \partial_x \kappa(\boldsymbol{r},t)
$$

\n- Diffusion stress:
$$
\tau_{\mathrm{d}}(\boldsymbol{r},t) = -Gb\frac{A}{\rho}\partial_x\rho(\boldsymbol{r},t)
$$
\n

• Flow stress:
$$
\tau_f(\mathbf{r}, t) = \alpha \mu b \sqrt{\rho(\mathbf{r}, t)}
$$

• Dimensionless fitting parameters: $D, \, A, \, \alpha$

I Groma, M Zaiser, FF Csikor, Acta Mater, 2003 I Groma, M Zaiser, PD Ispánovity, Phys Rev B, 2016

Correlation induced stress terms

• The *representative volume element* (RVE) cannot resolve internal correlations

unipolar walls composed of only one type of dislocation, either nega- \blacksquare Strength of a dinolarly disordered tilt walls, which are periodic arrays of edge dislocations

fluctuating state persists up to Fd55.0, when a new type of the SSS . When a new type of dynamics of \mathcal{S} pattern appears where the dislocations form continuously changing

that accommodate a tilt misorientation between two adjoining crys-two adjoining crystals. The development of low-misoriented tilt walls is suspected to be a precursor for the eventual formation of subgrains in heavily contained by the eventual formation of subgrains in heavily contained by

- In the middle of a dipolar wall: $\partial_x \rho = 0$ and $\partial_x \kappa < 0$
- The back-stress must be negative

Stochastic plasticity models

2D continuum equations

Assuming $\rho = \text{const.}$

Evolution equation for plastic strain $\dot{\gamma} = \rho b M_0 (\tau_{\rm mf} - \tau_{\rm f})$

> Considering τ_{f} as a *stochastic variable*

Journal of Statistica

Sham panem opon $t_{\rm r}$ model α Strain pattern upon shear

M Zaiser, P Moretti, J Stat Mech, 2005 Stochastic CA model for plasticity
S Sandfeld et al, J Stat Mech, 2015 $\ddot{}$ $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$

Avalanches, loading and finite size e↵*ects in 2D amorphous plasticity* 14

Avalanches, loading and \dagger

Implementation

$$
\partial_t \rho(\mathbf{r}, t) = -M_0 b \partial_x [\kappa \tau_{\rm mf} + \kappa \tau_{\rm b} + \rho \tau_{\rm d}]
$$

$$
\partial_t \kappa(\mathbf{r}, t) = -M_0 b \partial_x \left[\rho \tau_{\rm mf} + \rho \tau_{\rm b} - \rho \left(1 - \frac{\kappa^2}{\rho^2} \right) \tau_{\rm f} + \kappa \tau_{\rm d} \right]
$$

- CA implementation with extremal dynamics
- Dimensionless fitting parameters: $D, \, A, \, \alpha$
- Flow stress is a stochastic variable
- No phenomenological assumptions

PD Ispánovity, D Tüzes, P Szabó, M Zaiser, I Groma, arXiv, 2016

Evolution of density patterns

Characterization of pattern

• Cross-correlation of $+$ and $-$ sign dislocations

$$
C_{+-}(\Delta x, \Delta y) = \int \rho_+(x', y') \rho_-(x' + \Delta x, y' + \Delta y) dx' dy'
$$

$$
C_{+-}(\Delta x) := \langle C_{+-}(\Delta x, \Delta y) \rangle_{\Delta y} :
$$

Effect of parmeter D

• Order parameter: level of asymmetry in $C_{+-}(\Delta x)$

 $D = -0.6$

Effect of parmeter A

• Order parameter: level of asymmetry in $C_{+-}(\Delta x)$

Summary

- 2D continuum theory of dislocation dynamics
	- Derived analytically from the Eqs. of motion of discrete dislocations
	- It contains 3 dimensionless fitting parameters
	- There are no phenomenological assumptions, the gradient terms naturally emerge
- The 2D continuum theory properly captures the patterning and the strain response of 2D DDD simulations
- Inclusion of back-stress is necessary for pattern formation