

Dislocation avalanches: experiments and simulations Péter Dusán Ispánovity Eötvös University Budapest

Motivation

- Large stochastic fluctuations arise during the deformation of small (few um) crystalline samples
 - Makes predictable deformation impossible
- Power-law distributions characterize intermittency
- The question of universality is still open
 - What physical processes affect the critical behaviour and how?



Outline

- Intermittency in experiments on crystalline plasticity
 - Acoustic emission
 - Micropillar experiments
 - Nanoindentation pop-in events
- Simulations
 - Discrete dislocation dynamics
 - Stochastic models
- Simple 2D dislocation model
 - Anomalous system size behaviour
 - Extended cryticality

Crystal plasticity

Dislocations

- Linear lattice defects
- Carriers of plasticity
- They move due to shear stress
- They generate long-range shear stress field:

$$\sigma_{xy}(\mathbf{r}) = Gb \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$
$$= Gb \frac{\cos(\varphi)\cos(2\varphi)}{r}$$

 Complex spatio-temporal dynamics



3

Dislocation patterns



- Multitude of observed dislocation patterns
 - Fractal, periodic, etc.
 - Crucial impact on plastic properties
 - May lead to strain localization and failure of the material

H Mughrabi, F Ackermann, K Herz, STP675, 1979

H Mughrabi, T Ungár, W Kienle, M Wilkens, Philos Mag, 1986





Relevant lenght scales

- Atomic scale
 - Dislocation reactions and mobility
- Dislocation pattern
 - Scale proportional with $Q^{-1/2}$: principle of similitude
- Quenched disorder
 - Precipitates, point defects (solute atoms, vacancies, etc.)
- Grain size
 - Dislocations typically cannot penetrate boundaries
- Specimen size

Comments

- Thermal activation is not relevant at low temperatures
- Dislocation motion is dissipative

Small scales typically lead to hardening of the specimen

Stress-strain response

- Smooth curve for bulk samples
 - Large number of dislcoations
- Microplasticity
 - Deformation before yield
- Work hardening
 - Dislocations may multiply, annihilate and react during deformation
 - Pattern formation



Microplasticity



R.F. Tinder, J. Washburn, Acta Metall. (1964)

R.F. Tinder, J.P. Trzil, Acta Metall. (1973)

Crackling during bulk plasticity

- Zn single crystal (hcp)
- 'the strain curve of zinc crystals is not smooth, but consists of individual more or less sharp cracks'



Fig. 1. Die Versuchsanordnung.



Fig. 2. Sprunghafte Dehnung eines Zinkkristalls bei 80° C.

[Becker, Orowan (1932)]

Acoustic emission

- Detection of acoustic waves on the surface using a piesoelectric detector
 - The detected signal is characteristic to the source as well as the detector
 - The distance of the source matters
 - Burst-like vs. continuous signal





AE of ice

• Creep of ice (less than 0.1 MPa)

- $P(E) \propto E^{-\tau_E}$
- $\tau_E \approx 1.6$ (signal energy)
- $\tau_A \approx 2.0$ (signal amplitude)
- No cut-off





[Miguel et al., Nature (2001)]



of avalanches

can be located

ink bands

• They originate from a fractal sub-domain: *D* = 2.5





[Weiss et al., Science (2003)]

Effect of grain size

- Polycrystalline ice
 - Cutoff decreasing with grain size
 - Bimodal distribution due to secondary triggering across boundaries





[Richeton, Weiss, Louchet, Nat. Mater. (2005)]

HCP vs FCC materials

- Acoustic signal of fcc materials is mostly continuous interrupted with only few bursts
 - In fcc materials forest dislocations and junctions introduce a length scale: mild Gaussian fluctuations
 - In hcp no such scale exists: wild power-law fluctuations



[Weiss et al, PRL (2015)]

Conclusions of AE

- Relation between measured quantites and parameters of strain bursts somewhat unclear
- Time resolution for large samples or large strain rates may be a problem.
- Clear sign of criticality for bulk samples
 - Exponents suggest non-universal behaviour for different materials
- Internal length scales
 - No cutoff is detected for single crystals no information on length scale
 - System size dependence has not been studied AE only detectable for large samples

Micropillar compression

- Compression using a nanoindentor device
- Flat punch diamond tip
- The device contains a spring for displacement measurement
 - Machine stiffness comparable to sample stiffness





Micropillar compression

- Zn pillar oriented for single slip
- Diameter: 8 um
- Height: 24 um
- Displacment rate: 10 nm/sec
- Sudden activity on different slip planes (strain bursts, dislocation avalanches)
 - Unpredictable and localized both in time and space



Micron-scale crystal plasticity

- Size effects: smaller pillars are harder
- Stochasticity: smaller pillars are more random



D. M. Dimiduk et al., Acta Mater., 2005



Strain burst statistics

Previous investigations

 Strain burst sizes are power-law distributed:

• $P(s) \propto s^{-\tau} f(s/s_0)$

- τ: avalanche exponent
- *s*₀: avalanche cut-off
- f: cutoff function (e.g. $f(x) = \exp(-x)$)
- Experimentally measured exponents:
 - $\tau \approx 1.5, 2.0, 1.3$

Dimuduk et al., Science, 2006 Friedman et al., PRL, 2012 Zhang et al., EPL, 2012



Mean-field depinning

Compression of 7 Mo pillars

- Diameter: 800 nm
- Stress-binned statistics
- Scaling function:
 - $D(S, \tau) \sim S^{-\kappa} f_S(S(\tau_c \tau)^{1/\sigma})$
 - Mean field exponents obtained





[Friedman et al, PRL (2012)]

Issues with micropillar experiments

- Small number of events: large statistical errors
- Yield stress of individual pillars strongly fluctuates
- Very few avalanches in the elastic regime
- The results are very sensitive to experimental details
 - System size
 - For nanopillars new defromation mechanisms
 Parallel tip and sample surface
 Surface degradation duew to FIB

 - Deformation and sampling rate
 - Non-uniform pillar shape
 - Machine stiffness





Role of grain boundaries

Low angle grain boundary



Coherent grain boundary



[Imrich et al., Acta Mater. (2014)]





Effect of microstructure

- Avalanche distribution unaffected by original dislocation structure
- Sampling rate affects the exponent



[Maass, Derlet, Acta Mater. (2018)]

Effect of irradiation

- Self-ion irradiated <111> Ni:
 - Smoother response for small doses
 - Large fluctations for high doses



[Zhao et al, Acta Mater (2015)]



Nanoindentation: pop-in events

- First pop-in events in Mo
- Weibull distribution describes well the pop-in stresses



[Phani, Johanns, George, Pharr, J. Mater. Res. (2013); Derlet, Maass, J. Appl. Phys. (2016)]



Conclusions of experiments

- Clear sign of critical behaviour
 - Power-law distributions
 - Technologically important to understand small-scale deformation
- Internal scales seem to affect the avalanche distribution
 - Grain boundaries, quenched pinning
- Measured data suffer from
 - Small datasets
 - Experimental difficulties
 - Too small samples
- One cannot conclude regarding universality

Discrete dislocation

 $P(s) \propto s^{-\tau} f(s/s_0)$

- 3D DDD simulations on Al
- Mean-field exponent
- Behaviour of the cut-off:



- b: Burgers vector
- E: Young modulus
- L: system size
- Θ: strain hardening
- Γ: effective stiffness of the machine-sample system



[Csikor et al, Science, (2007)]

2D DDD

- Edge dislocations in single or multiple slip systems
 - Sources and obstacles







ε_{zz}

-0.1

-0.2

-0.3

-0.4

-0.5

-0.6

-0.7

-0.8

-0.9 -1





2D DDD

- Weak sources (left): cutoff dependent on sample size
 - Size effect; larger events for thin samples, $\tau = 1.5$
- Strong sources (right): constant cutoff
 - No size effect; event distribution independent of size; $\tau = 1.9$



[Papanikolaou, Song, van der Giessen, J. Mech. Phys. Solids (2017)]

Representation of inhomogeneities

- The microstructure of the material is inhomogeneous
 - Dislocation patterns
 - Random impurities
 - Grain structure
 - The local strength (yield stress) is inhomogeneous in space
- Representing internal disorder
 - Via a local yield threshold
 - RVE size comparable to the scale of disorder
- Deformation will always occur at the 'weakest' site







Stochastic plasticity model

Simple local shear deformation:

- Shear stress increases above the local yield threshold
- Plastic deformation: Slip along a single plane
- The local yield threshold changes due to the changed microstructure
- The slipped cell generates $1/r^2$ type elastic stress (Eshelby inclusion problem)



Stress field of a dislocation dipole



• Shear stress field for large distances: $\sigma_{xy}(x,y) = \frac{\cos(2\varphi)}{r^2}$

Depinning in the stochastic model

• Cutoff divergence as external stress ($\tau_{\rm ext}$) tends to the critical threshold ($\tau_{\rm c}$)



- Dislocation density is constant: no patterns
- Length of RVE? Is there an internal correlation length?

[Zaiser, Moretti, JStat (2005)]

Avalanches during depinning



- Avalanche size s is the area swept
- The size distribution depends on the force (F) and system size (L) The cutoff s₀ diverges at

force $F = F_{c}$:

$$s_0(F) \propto |F - F_c|^{-\alpha}$$

The average avalanche size $\langle s \rangle$ diverges at F_c Finite size effects near F_c :

$$F_{\rm c}(L) = F_{\rm c}(\infty) + aL^{-1}$$

Mean-field case:

• *τ* = 1.5

2D dislocation models

2D DDD

- Parallel edge dislocations in single slip
- Periodic boundary conditions
- Number of dislocations: N
- Sign of dislocations: $s_i = \pm 1$
- Stress-field of an individual dislocation: σ_{xy}
- Overdamped motion:

$$\dot{x}_i = s_i \left[\sigma_{\text{ext}} + \sum_{i=1}^N s_j \sigma_{xy} (\boldsymbol{r}_i - \boldsymbol{r}_j) \right]$$





Problem formulation

- Energy of a straight edge dislocation: $E = Gb \uparrow 2 \ln L / r \downarrow c$
 - $G = \mu/4\pi(1-\nu)$, L: crystal size, r_c : core radius, b: Burgers vector

- Energy density of N randomly positioned straight edge dislocations:
 - The stored energy density is system size dependent
 - The width of the Bragg peaks is also proportional to In(L)



 Dislocation systems cannot be completely random: there must be spatial correlations

M. Wilkens, 1969

Relaxation from a random initial configuration



Small-scale configurations

- Equilibrium dislocation configurations are not random: they are characterized by short-range ordering
- Equilibrium positions of a dislocation pair:
 - Opposite sign: dislocation dipole



• Same sign: dislocation wall



Spatial correlation functions

- Spatial correlation functions: dislocation density around a randomly chosen dislocation :
 - d_{+-} : relative of the opposite sign dislocations
 - d_{++} : relative of the same sign dislocations, $d_{++}(0,y) \propto |y|^{-1.5}$



(Debye-)screened stress field

- Elastic energy density of a random dislocation arrangment is superextensive
- Local correlations screen the average stress around each dislocation



[Groma et al., PRL, (2006)]

Relaxation from a random initial state



- Average absolute velocity: $\langle |v(t)| \rangle \propto t^{-lpha}, \quad lpha \approx 0.87$
- The cut-off t_c diverges with system size



F. F. Csikor et al., JSTAT, 2009; P. D. Ispánovity et al., PRL, 2011

Velocity distribution & scaling

- P(v,t): Distribution of dislocation velocities v at time t
 - Inverse cubic tail (from theory as well)
 - Tends to a δ -function as t
- Scaling property: $P(v,t) = t^{\alpha} f(t^{\alpha} v) \implies \langle |v(t)| \rangle \propto t^{\alpha}$

= 0.4

 10^{-1}

 $\mathbf{v} \cdot t^{\alpha}$

10⁰

v-3

 10^{2}

 10^{1}



P. D. Ispánovity et al., PRL, 2011

Relaxation due to a small applied stress

• $\tau_{\rm ext} < \tau_{\rm c}$ • N = 128





Strain rate evolution

Strain rate:

- $\dot{\gamma}_{
 m pl} \propto t^{-\delta}$ (Andrade creep law)
- $\delta \approx 0.64$
- cut-off diverges with sytem size

Velocity distribution:

 Both the symmetric and asymmetric part follows scaling

P. D. Ispánovity et al., PRL, 2011



Summary

- Relaxation at different set-ups show slow, power-law relaxation everywhere below the yield stress
- The cut-off time diverges with the system size
- The velocity distributions obey simple scaling relations

- There is no time scale in the system (except for the scale due to finite system size)
- The system behaves as if it was critical everywhere below the yield stress

Single slip plastic quasistatic shear in 2D



Strain burst distributions

- Avalanche size s is the total area swept
- System size: $L = \sqrt{N}$





Dependence on the applied stress (N = 4096)

Dependence on the system size ($\sigma_{\rm ext} = 0.316$)

Ispánovity, Laurson, Zaiser, Groma, Zapperi, Alava, PRL, 2014

Cutoff scaling

Strain burst size distribution:

 $P(s) \propto s^{-\tau} \exp(-s/s_0)$

Cutoff scaling:

$$s_0(\sigma_{\rm ext}, N) \propto N^{\beta} \exp(\sigma_{\rm ext}/\sigma_0)$$

Parameters:

- Avalanche size exp.: $\tau \approx 0.97$
- System size exponent: $\beta \approx 0.36$
- Stress scale: σ_0



Ispánovity, Laurson, Zaiser, Groma, Zapperi, Alava, PRL, 2014

Comparison of models

Cutoff behaviour: $s_0(\sigma_{\rm ext}, N) \propto N^\beta \exp(\sigma_{\rm ext}/\sigma_0)$



Continuous model

CA model with ED

CA model with RD

Model	τ	β	σ_0	
Continuous	0.97±0.03	0.36±0.04	0.07±0.01	•
CA with ED	1.00±0.03	0.36±0.02	0.116±0.004	•
CA with RD	1.02±0.01	0.44±0.01	0.122±0.002	-

•
$$\tau \approx 1.0$$

• $\beta \approx 0.4$

Average avalanche shape

- Avalanche shape following the Eshelby directions
- 1/r decay
- No cutoff in the avalanche shape



Ispánovity, Laurson, Zaiser, Groma, Zapperi, Alava, PRL, 2014

Non-depinning behaviour



 $\langle \gamma \rangle = L^{2\beta-2} \exp(\sigma_{\text{ext}} / \sigma_0)$

Further evidence

- Glassy avalanche distributions in 3D DDD simulations
- Power-law distributions for the local yield stress (in 2D and 3D)
 - Only one dislocation or a local region is excited
 - The exponent θ
 dependes on
 loading rate

[Lehtinen, Costantini, Alava, Zapperi, Laurson, PRB (2016)] [Ovaska, Lehtinen, Alava, Laurson, Zapperi, PRL (2017)]

(b)

60

х

40

80





Effect of quenched pinning



- jamming \rightarrow pinning \rightarrow Gaussian dynamics
- A gap in the local threshold distribution



strengt Strong pinning, non-critical dynamics Disorder Pinning Sustained plastic flow Jammed **External stress Conventional DDD** 10 $\frac{9}{8}$ $(s) = 10^{-1}$ 0.004 0.002 $\circ \sigma_{ext} = 0.175 \Box \sigma_{ext} = 0.325$ $\circ \sigma_{ext} = 0.475 \Delta \sigma_{ext} = 0.625$ 10-3 $\triangleleft \sigma_{ext} = 0.775 \nabla \sigma_{ext} = 0.925$ $\triangleright \sigma_{ext} = 1.075 + \sigma_{ext}$ 10^{-2} 10^{-3} 10^{-4} 10^{-1} 10^{0}

Summary

- Pure dislocation systems exhibit extended criticality
 - There is no correlation length associated with dislocation structure
 - Slow relaxation
 - The avalanche size diverges at every applied stress level
- Plastic yielding in general cannot be described in terms of a depinning transition
- Robust: recovered in 3D simulations as well
- This picture may be compatible with experiments on pure hcp or fcc materials
- Introduction of internal length scale changes the picture
 - Depinning or Gaussian fluctuations

Outlook

Questions

- How does the transition from jamming to depinning happen?
 - System size dependence
 - Is it possible to get into extended crytical region by loading?
- What influences the exponent?
- How does strain hardening and other phenomena affect universality?
- How to go to higher scales? What is the RVE?

• Work in progress

- Implementing finite boundaries
- New algorithms to allow for larger systems/less numerical noise
- Get closer to experiments: multiple slip, Peierls stress
- Local yield threshold distributions

Statistical analysis of stress-strain curves



- Stress values for a given plastic strain level
- Distribution of these stress values

Average stress-strain curves

• Average and standard deviation of stress strain curves



There is only a negligible size effect!

Stress sequence statistics

- The stress-strain curve is a sequence of discrete stress and strain values:
 - au_i : shear stress at the ith event
 - γ_i : shear strain at the ith event
- Distribution of strain increments $\Delta \gamma_i = \gamma_i \gamma_{i-1}$ has been discussed
- What is the distribution of τ_i ?



Distribution of τ_1



For larger systems stress values get smaller:

 $\langle \tau^{(1)} \rangle \propto 1/L$

 Cumulative distribution is a Weibull:

$$\Phi^{(1)}(\tau_1) = 1 - \exp\left(-\left(\frac{\tau_1}{\lambda}\right)^{\nu}\right)$$

• Shape parameter: $v \approx 1.4$

Background of the Weibull distribution

- A chain consists of independent links
- If the asymptotic ($\tau \rightarrow 0$) failure distribution of **one link** is:

$$\Phi(\tau) = \left(\frac{\tau}{\tau_0}\right)^{\nu} \implies P(\tau) = \Phi'(\tau) = \frac{\nu}{\tau_0} \left(\frac{\tau}{\tau_0}\right)^{\nu-1}$$

then the failure distribution of the chain of M links is

$$\Phi^{(1)}(\tau^{(1)}) = 1 - \exp\left(-\frac{1}{M}\left(\frac{\tau^{(1)}}{\tau_0}\right)^{\nu}\right)$$



Stress sequence

- What about the statistics of τ_i ?
- Mean: $\left\langle \tau^{(i)} \right\rangle = \frac{\tau_0}{M^{1/\nu}} \frac{\Gamma(i+1/\nu)}{\Gamma(i)} \approx \tau_0 \left(\frac{i}{M}\right)^{1/\nu}, \text{ if } i \ge 5$ • Standard deviation: $\Delta \tau^{(i)} \approx \frac{\tau_0}{i^{1/2}} \left(\frac{i}{M}\right)^{1/\nu}, \text{ if } i \ge 5$



Size dependence

- How does the number of links M depend on the system size?
- Assumption: $M \propto L^{\xi}$
 - If links are homogeneously distributed, then $\xi = 2$.

$$\left\langle \tau^{(i)} \right\rangle \approx \tau_0 \left(\frac{i}{M}\right)^{1/\nu} = \frac{\tau_0}{L^{\xi/\nu}} i^{1/\nu}$$



- From the fit $\xi / \nu \approx 1.2 \Rightarrow \xi = 1.2 \cdot \nu \approx 1.7$
- The numer of links grows subextensively with the system size

Plasticity model

- Stresses τ_i are an independent random sequence drawn from a Weibull distribution with shape parameter v.
- Strain increments are independent random variables with finite moments:



• Average stress-strain curve:



- $\langle \tau \rangle \propto \left(\frac{L^{\eta}}{L^{\xi}} \right) \langle \gamma \rangle$
- Standard deviation of stresses: $\Delta au \propto L^{-\xi/2}ig\langle\gammaig
 angle$



 γ_i

Average stress-strain curves

Average and standard deviation of stress strain curves



Distribution of stress values at a given strain

- Stresses at a given strain for different realizations are normally distributed
- The standard deviation decreases with increasing system size



Conclusions, outlook, acknowledgements

Conclusions

- The concepts of the stochastic model of Zaiser are in agreement with 2D DDD
- A simple plasticity model of independent avalanches gives a good description of the microplastic part of the stress-strain curves
- A method has been proposed to set the yield threshold distribution in the stochastic model (multiscale modelling)

Acknowledgements

- European Commission, Marie Curie CIG StochPlast 321842
- Hungarian Scientific and Research Fund OTKA PD-105256, OTKA K-105335