Using Stochastic theory for RF breakdown analysis

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Plasticity of collective dislocation ensembles from stochastic to mean field

ELSEVIER Materials Science and Engineering A322 (2002) 194–216 www.elsevier.com/locate/msea

Constitutive description of dynamic deformation: physically-based mechanisms

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- Plastic response - controlled to a large extent by dislocations (slip, twinning)
- The stochatic nature of the underlying dislocations reactions is translated through average rates to a constitutive relation = deterministic relation between stress , strain, strain rate etc.

$$P_i = \nu_i / \nu_0 \rightarrow \nu_i \sim \nu_0 \exp\left(-\Delta G / kT\right)$$

- Using Orowan equation – dislocation motion to strain (Δl between dislocation barriers, b –burgers vector)

$$\dot{\gamma} \sim \rho_d b \underbrace{\frac{\Delta l}{\Delta t}}_{V_{dis}}$$

- Assume V>>barrier crossing time thereor Δt between crossing is given by $1/\nu_1$

$$\dot{\gamma} = \dot{\gamma}_0 \exp\left(-\Delta G / k_B T\right) \longrightarrow \Delta G = k_B T \ln\left(\dot{\gamma}_0 / \dot{\gamma}\right)$$

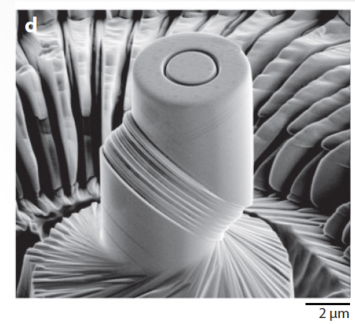
- By assuming a functional form for ΔG one gets a constitutive link between stress, T and strain rate.

Also: Steck and Gerdes, acta mechanica, (1997)

Dislocation mediated – self organized criticality

Plasticity of Micrometer-Scale Single Crystals in Compression

Michael D. Uchic,[1] Paul A. Shade,[2] and Dennis M. Dimiduk[1]



Single crystal micro-pillar compression:

Dislocation mediated intermittent flow - size effects, hardening.

Dislocation density inside a plane as a controlling parameter.

Direct quantitative analysis of strain bursts (~20 micron).

Intermittency characterized by a universal Power law burst PDF

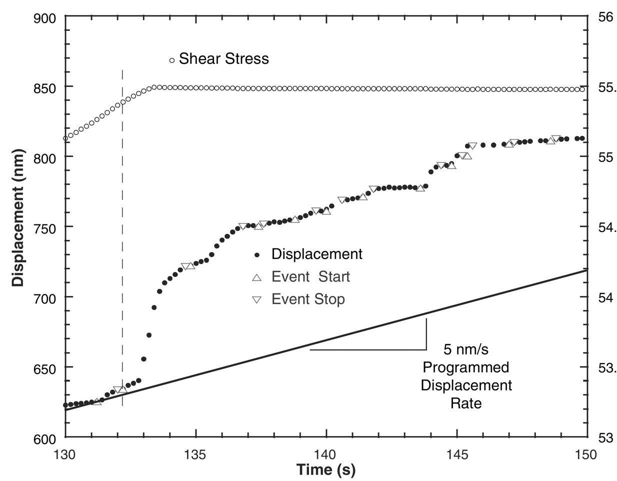
Acoustic emissions:

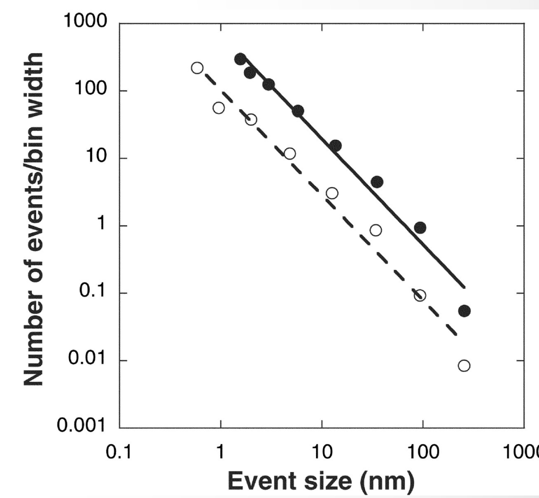
Similar + space and time coupling between events

(Weiss & Marsan, Scjence 2003)

Earthquakes show similar PDF and spatio-temporal correlation

(Kagan, Geopgysical J. (2007)





Uchic, Shade & Dimiduk, Annual Review of Materials Research (2009).

Dimiduk, Woodward, LeSar & Uchic: "Scale-Free Intermittent Flow in Crystal Plasticity." Science (2006) 1188.

Using dislocation dynamics to reproduce PDF

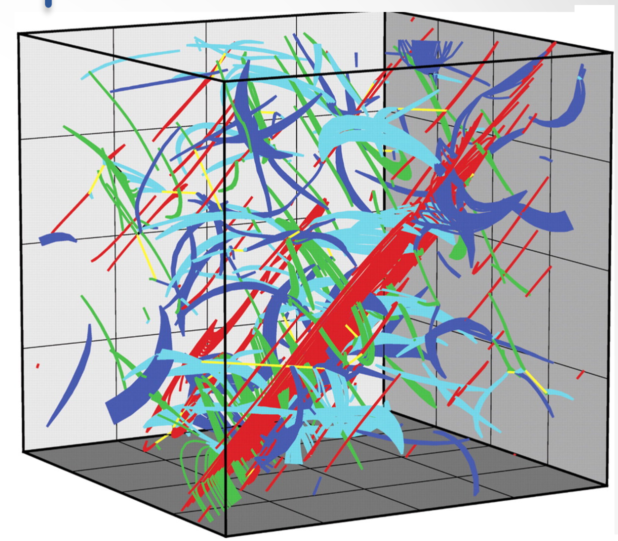
- 3D dislocation dynamics reproduce strain burst scaling $P(s) = Cs^{-\tau}\exp\left[-\left(s/s_0\right)^2\right]$

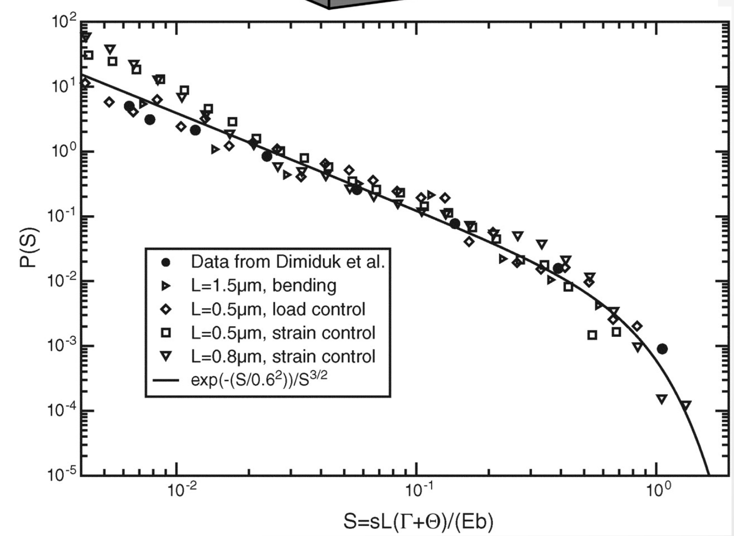
- where C is a normalization constant, τ is a scaling exponent, and s_0 is the characteristic strain of the largest avalanches.

- Intermittency – as a result of dislocation Interactions. Stochastic nature a result of varying initial conditions.

- Avalanche is a 2D event, with an upper cutoff due to structure and work-hardening. Strain is limited to about 10^-6 in a cm size sample.

- Recently (Chen, choi, papanikolaou & Sethna 2010 to 2013): scaling of structures using an advanced CDD code.





Csikor, Motz, Weygand, Zaiser & Zapperi, "Dislocation Avalanches, Strain Bursts, and the Problem of Plastic Forming at the Micrometer Scale" . Science (2007)

Spatial phase field modeling

- Using deterministic spatial model:
  - spatial phase filed leads to complex geometrical and topological transitions: forest hardening, multplication, slip bands
    Koslowski, Cuitino and Ortiz, J. Mech & Phys solids 2002
  - Complex governing equations. Leads to intermittent response and reproduces experimentally observed avalanche scaling laws.
  - Behavior reproduced by moving from a fully 3D system to a 1D "in slip plane" model. (Koslowski *phil. Mag.* 2003)
- Modifications
  - Modifications – such as: Introduction of Explicit fluctuations as a function of dislocations density (Zaiser & Moretti, J stat Mech 2005)
  - The main aim here is analytical tractability

Review of all methods:

Current theoretical approaches to collective behavior of dislocations

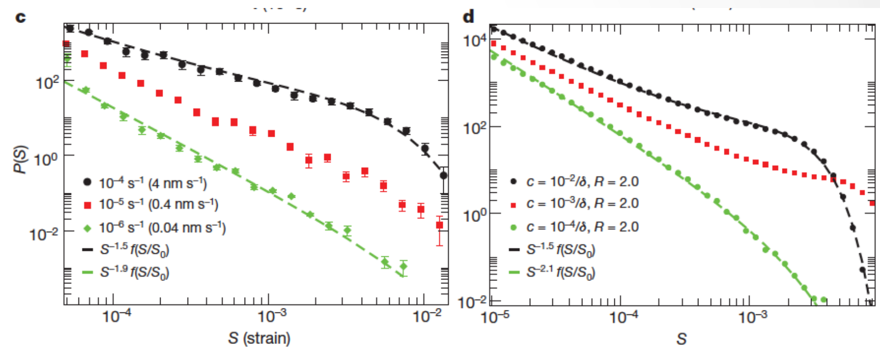
G. Ananthakrishna* Physics Rep. (2007) 113

Mean field models for critical depining

Quasi-periodic events in crystal plasticity and the self-organized avalanche oscillator

Stefanos Papanikolaou[1], Dennis M. Dimiduk[2], Woosong Choi[3], James P. Sethna[3], Michael D. Uchic[2], Christopher F. Woodward[2] & Stefano Zapperi[4,5]

- Reproduce strain rate variation by modifying the mean field picture to include a competing relaxation mechanism. This lead to oscillation in avalanche size. (nature, 2012)



PRL 109, 105702 (2012) PHYSICAL REVIEW LETTERS week ending 7 SEPTEMBER 2012

Distribution of Maximum Velocities in Avalanches Near the Depinning Transition

Michael LeBlanc,[1] Luiza Angheluta,[1,2] Karin Dahmen,[1] and Nigel Goldenfeld[1]

- Using a mean field model for interface depining and by solving Fokker-Planck eq. reproduced the power law decay of avalanche size and maximal velocity

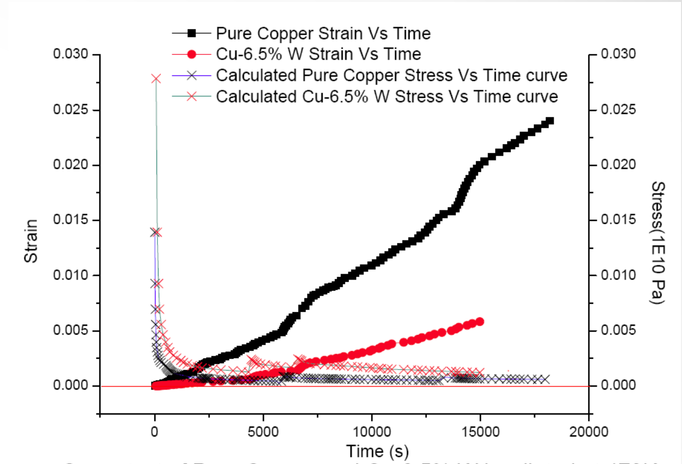
$$\frac{dV}{dt} = -kV + F_c + \sqrt{V}\xi(t)$$

Relation to creep model

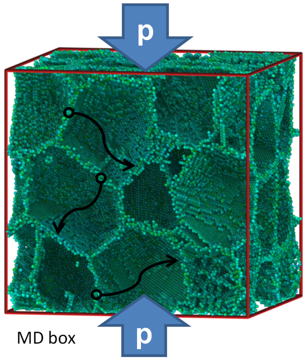
- In nano-crystalline systems radiation induced creep (due to point defect generation) can be significantly reduced. (Tai, Averback, Bellon and Ashkenazy Scripta Mat. (2011))

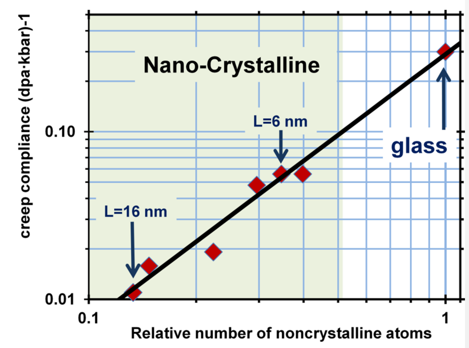
- We showed (using mean field model and atomistic simulations) that de-pining in grain boundaries by point defects can lead to radiation induced creep and reproduced experimental dependency. Controlling these de-pining events may allow increased IIC.
(Ashkenazy & averback Nanoletters 2012)

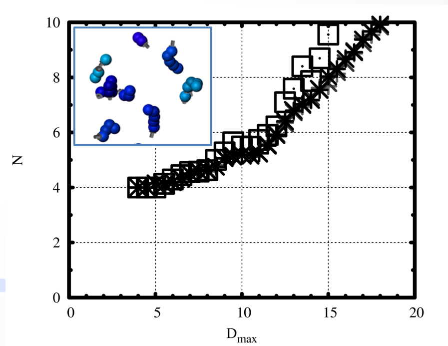
- Response in GB to external stress shows a distribution of depining events.



Creep test of Pure Copper and Cu-6.5% W irradiated at 473K







What are we trying to do…

- Use stochastic theory to allow for:
  - transferability of failure scenario analysis (across drive conditions)
  - Identify controlling mechanisms
  - Define critical experiments - model development / verification

  Such models serve as a link between the microscopic, short time scale problem which is accessible via simulation to the measured system to the real life scenario.

For now – demonstrate the basic method using a "spherical horse" model.

Not trying to do (at this stage):

Create a comprehensive consistent microscopic model

Describe the "real" mechanism at work

Link to "state of the art" DDD model.

PHYSICAL REVIEW SPECIAL TOPICS - ACCELERATORS AND BEAMS **15**, 071002 (2012)

Defect model for the dependence of breakdown rate on external electric fields

K. Nordlund and F. Djurabekova

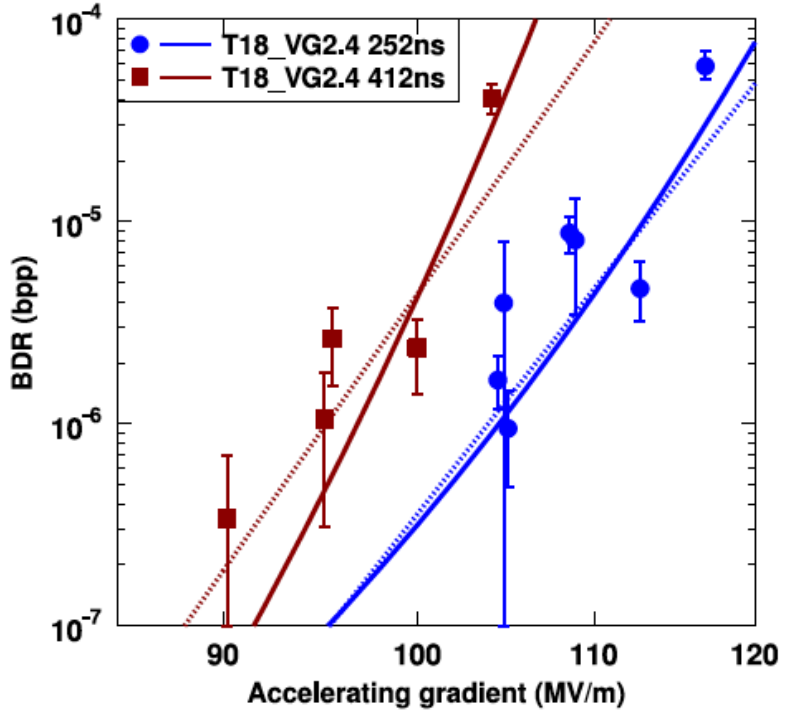


FIG. 4. Measured dependences of R_{BD} (in units of breakdown per pulse, bpp) versus electric field for the T18 accelerating structure [33,43] and fits of our model (solid lines) as well as power laws (dashed lines) to the data.

$$\frac{1}{\tau_{RBD}} \approx \exp\left[E^2 \Delta V / \left(k_B T\right)\right]$$

Formulation of a "well-mixed" 0d model

- Assumptions:
  - Breakdown currents are driven by formation of surface extrusion/intrusions.
  - Surface protrusions are formed due to multiple dislocation reaction leading to local
  - Sub-breakdown surface protrusion are not identified (Is that true?). Therefor we assume that gradual protrusion accumulation does not control breakdown:
    - surface relaxation, interaction between various slip systems, protrusion-dislocation interaction…
    - Field conditions are translated to an applied stress (AC thermal gradients ~ 100 Mpa, dc?)

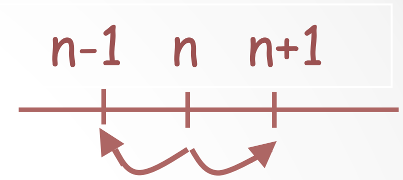
- Suggested controlling parameter - the number of mobile dislocations inside a band.
  - If large amount of dislocations reach the surface in unison – an instant extrusion/intrusion may lead to breakdown.
  - We avoid spatial interaction and assume gain-loss dynamics inside a specific band.

General gain-loss type Markovian processes

Rates for transition between states

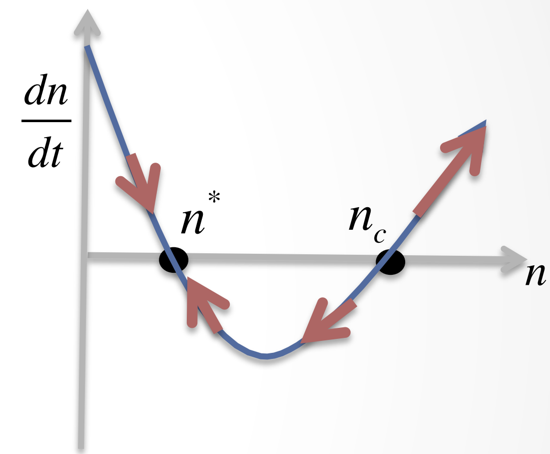
$$n \xrightarrow{\rho_n^+} n+1$$

$$n \xrightarrow{\rho_n^-} n-1$$



The master equation

$$\dot{P}_n = \rho_{n-1}^+ P_{n-1} + \rho_{n+1}^- P_{n+1} - \left(\rho_n^+ + \rho_n^-\right) P_n$$



can lead to bifurcation:
a metastable state and a critical one.

We look for the quasi-stationary probability distribution function
And the probability to cross the critical point (reach extinction)

Approximate solution based on WKB theory with 1/N being the small parameter.

$$\dot{P} = 0 \quad \Rightarrow \quad P(n) \equiv P(\rho N) \sim e^{-N[S(\rho)+O(1/N)]}$$

Assaf and Meerson, PRE 2010

"Minimal" model

- Define the "in-plane" density (in units of 1/nm).
- External stress (due to temp gradient on surface), range of 0.1 Gpa.
- Mobile dislocations can increase in number due to stress gradient (the driving force) as well as thermal activation of the multiplication reaction

$$\frac{d\rho^+}{dt} = v_0 \mu A(\sigma(\rho))^k e^{-(\phi_0 - \sigma\Omega)/k_B T}$$

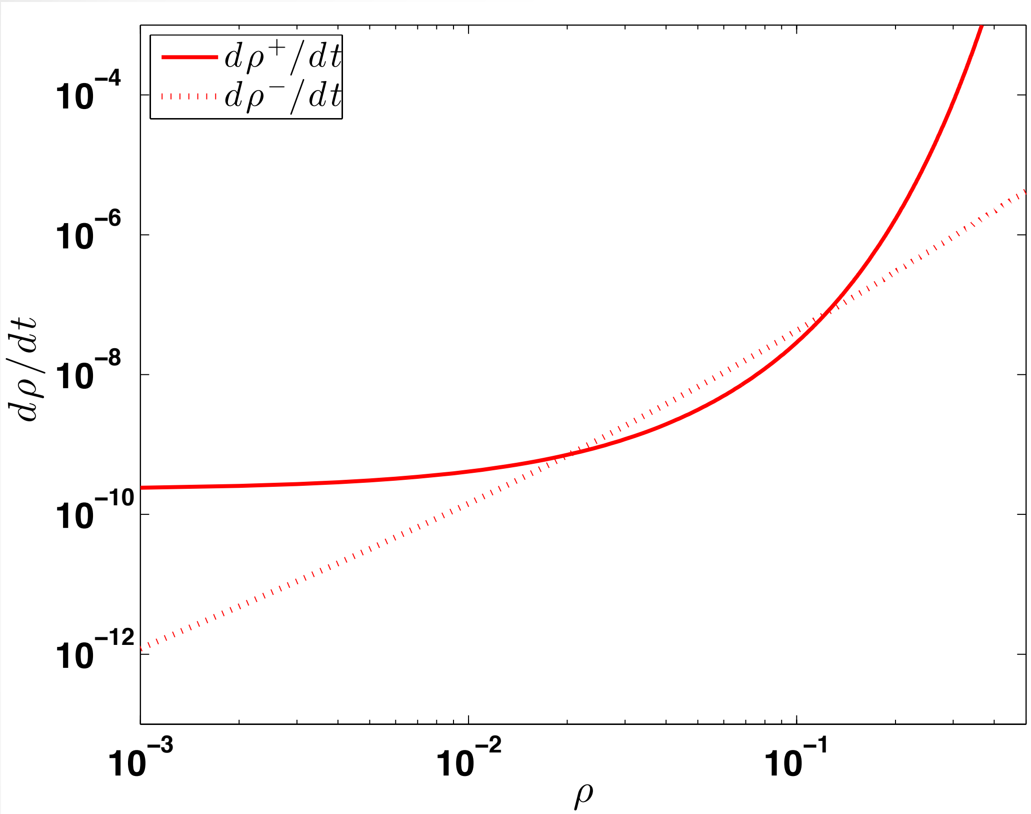
- Moving dislocations can become sessile at:
  - Pre-existing barriers (concentration - C)
  - "collisions" with other moving dislocations

$$\frac{d\rho^-}{dt} = \rho V(\sigma)c + \rho 2V(\sigma)\rho$$

- Properties dependence:
  - Velocity increase with stress, independent of the number of moving dislocations
  - Stress increase with dislocation content

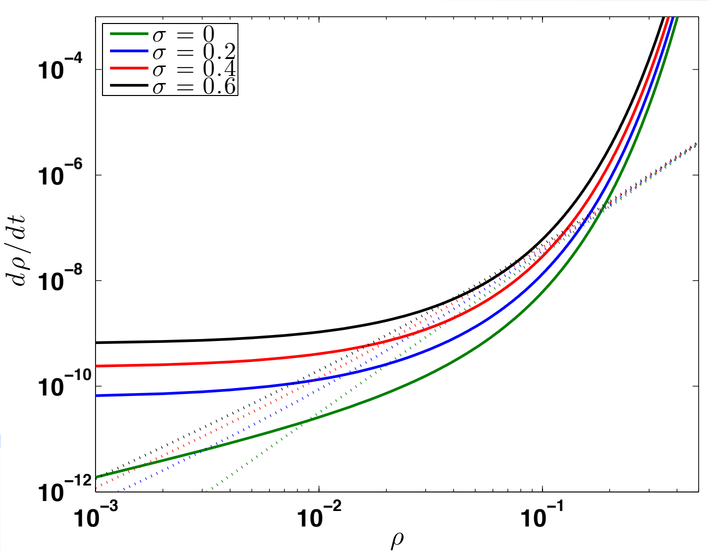
$$\sigma = \sigma_E + \mu\rho b \qquad V = Bv_0 b^2 \sigma$$

Model characteristics

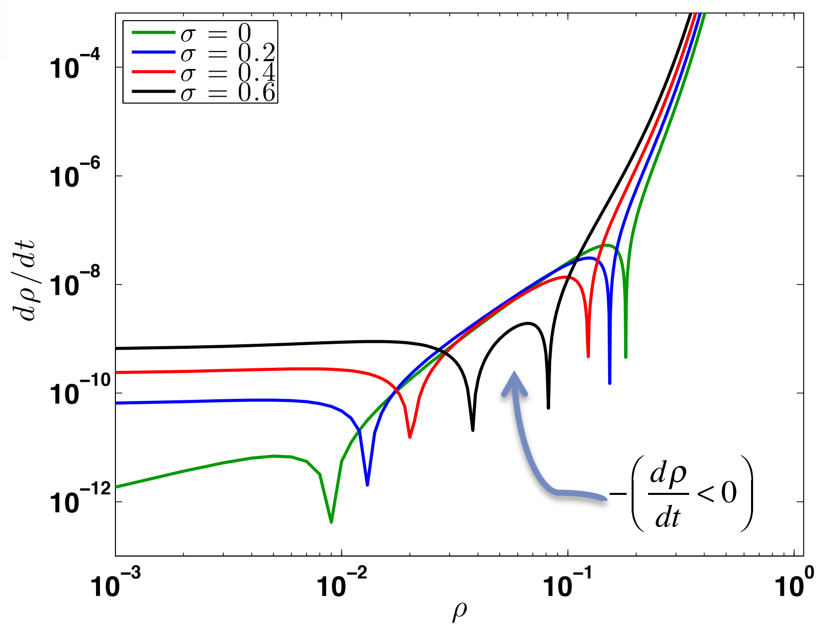


Stable point:
Dislocation generation and annihilation identical

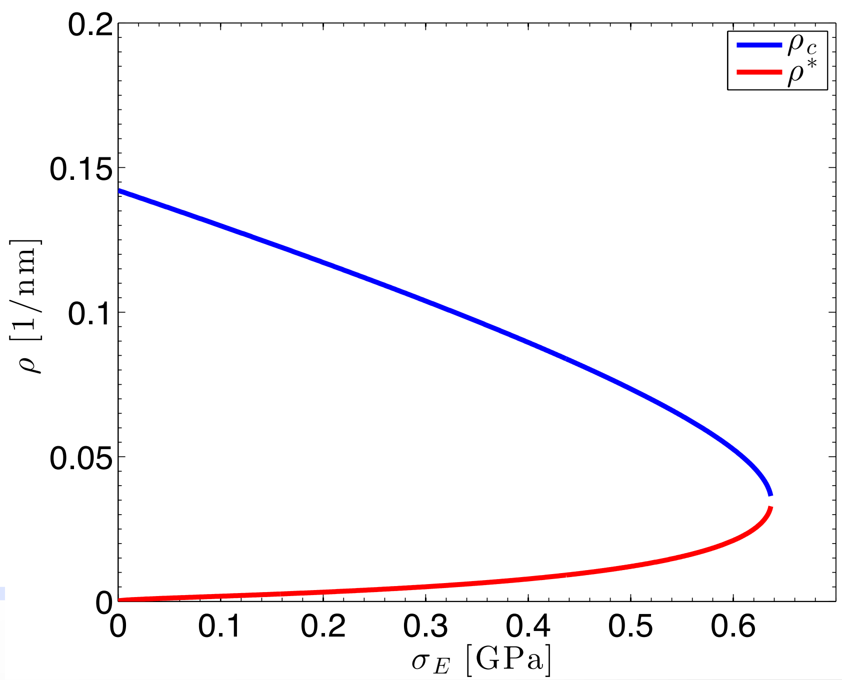
Critical point – threshold for dislocations avalanche



Low stresses:
Mobile dislocation density remains in Metastable solution.
Dynamic barrier decreases with increasing stress.



Up to a critical stress – bifurcation to two solutions.
Above it – no stable solution.



Define : $$s(\rho)=-\int_{\rho}\ln\frac{\rho^{+}(x)}{\rho^{-}(x)}dx$$

Fro (k=2): $$s(\rho)=-\rho\ln\left[\frac{\rho^{+}(\rho)}{\rho^{-}(\rho)}\right]-\frac{\sigma_E}{b\mu}\ln\left[\sigma(\rho)\right]+\frac{c}{2}\ln(c+2\rho)-\rho\left(1-\frac{\rho b\mu\Omega}{2k_BT}\right)$$

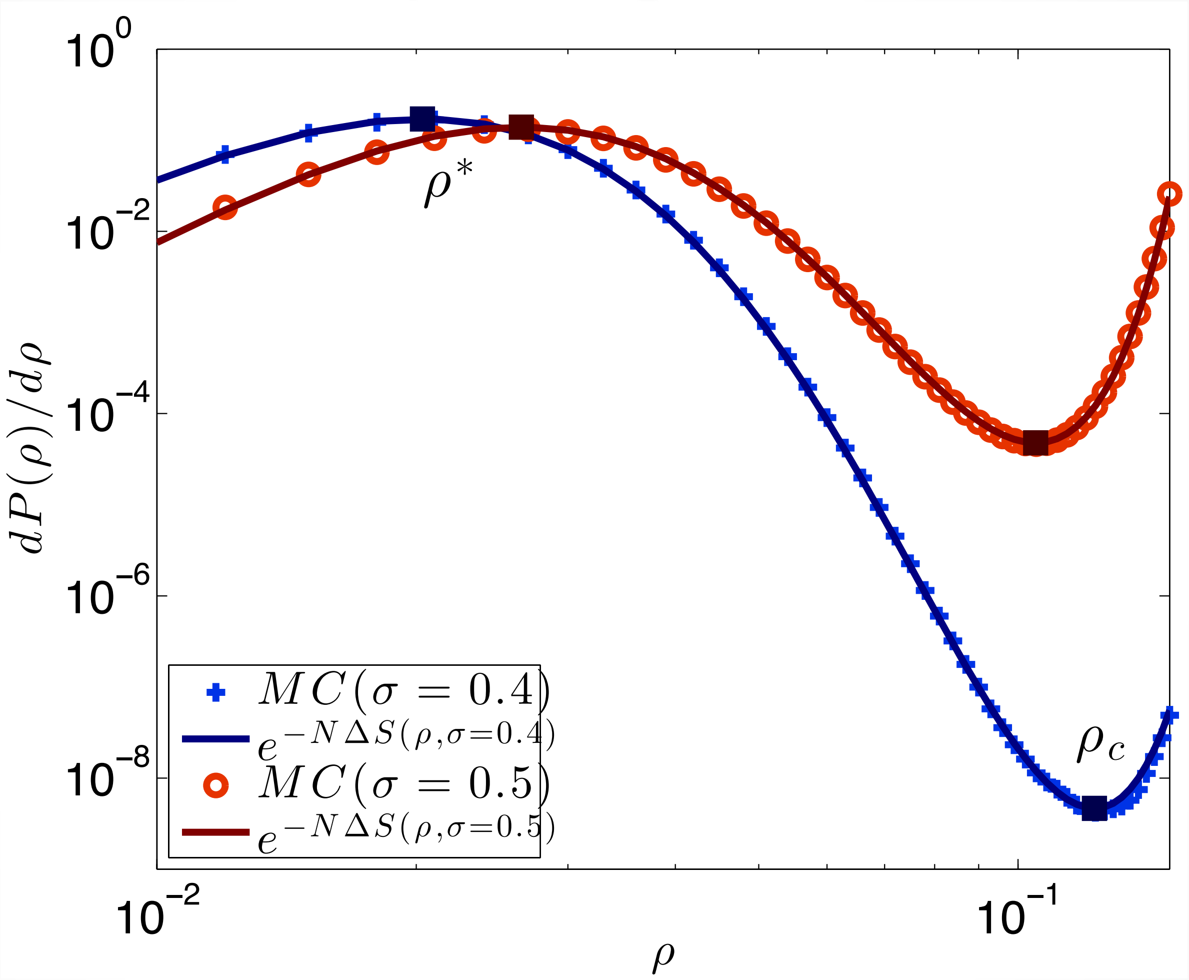
Using*: $$P(n=N\rho)=P(\rho)\sim e^{-Ns(\rho)}$$

Leads to $$P(\rho)\propto\left[\frac{\rho^{+}(\rho)}{\rho^{-}(\rho)}\right]^{N\rho}\frac{\left[\sigma(\rho)\right]^{N\sigma_E/b\mu}}{(c+2\rho)^{Nc/2}}e^{N\rho\left(1-\frac{\rho b\mu\Omega}{2k_BT}\right)}$$

And the normalized PDF $$P(\rho)=\underbrace{\sqrt{\frac{S''(\rho^{*})}{2\pi N}}}_{P(\rho^*)}e^{-N[s(\rho)-s(\rho^{*})]}$$

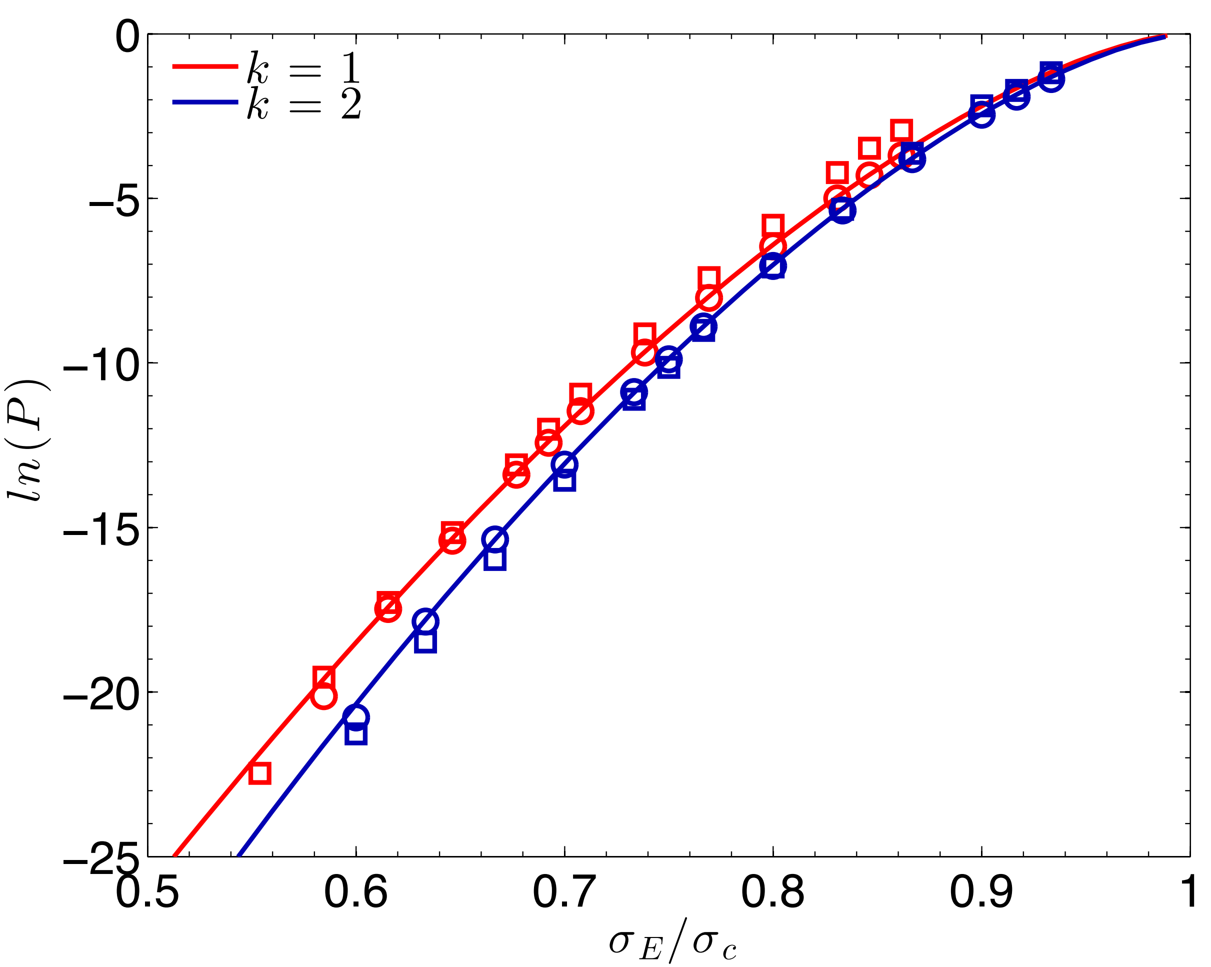
*Assaf and Meerson, Phys Rev. E 21116 (2010)

Comparing PDF



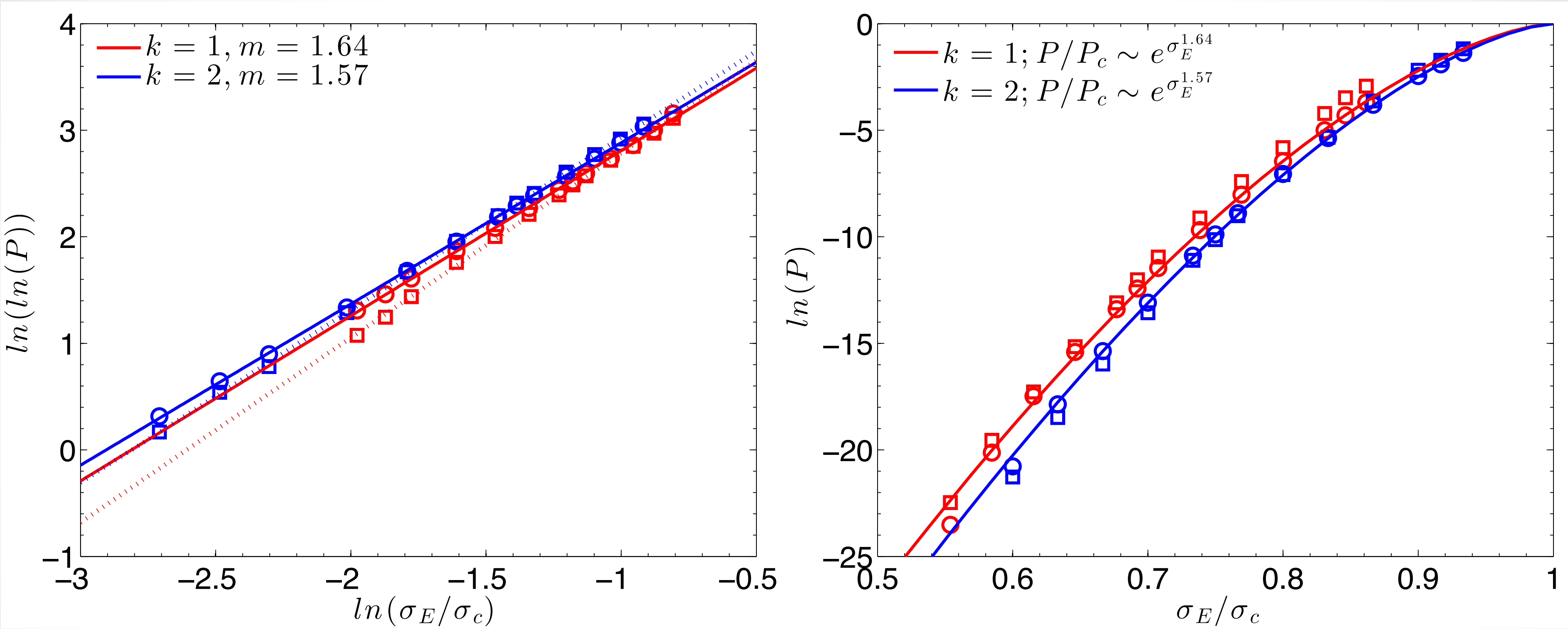
- Analytical analysis reproduces full PDF.

Comparison with simulation results - BDR



- Analytical solution for relative probability to reach critical point.
- Normalized probability and rate for reaching the critical state.

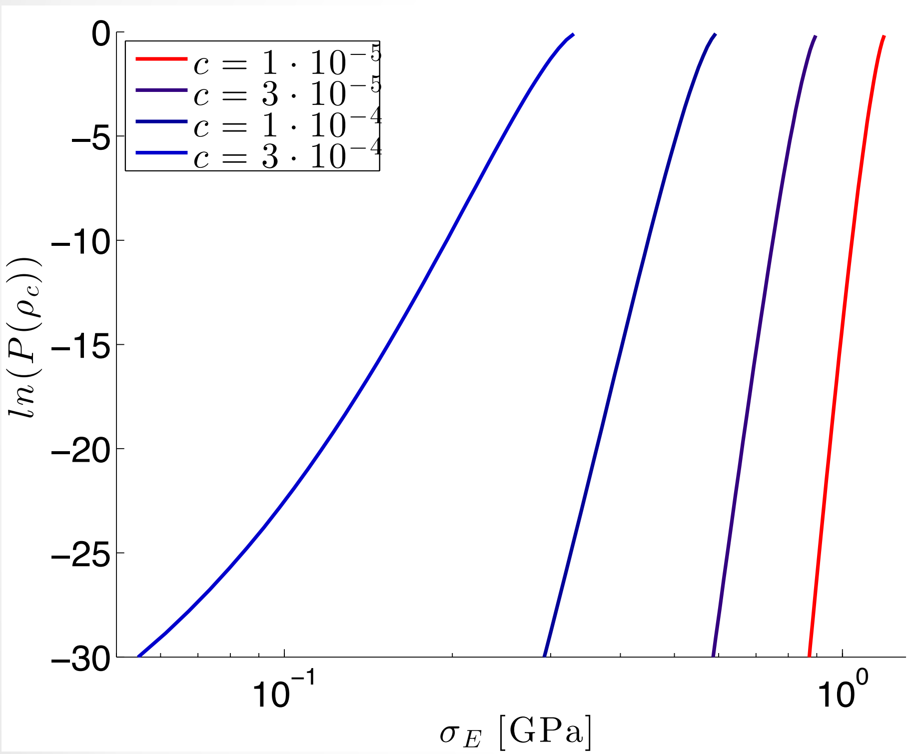
Fitting to reproduce observed BDR



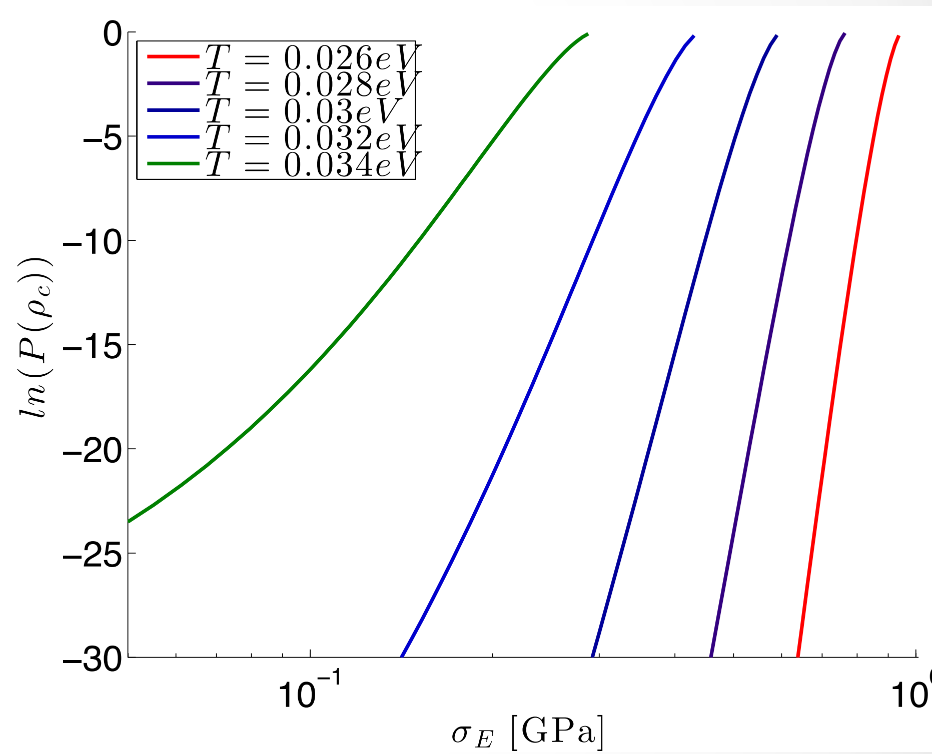
- Within range from fit to experimental $P \sim \frac{1}{\tau} \sim \exp\left(\sigma_E^{1.6}\right)$

Other dependencies

Employ analytical solution to various scenarios



Dependency on mobile dislocation generation pre-factor



Temperature dependence.

PRE-breakdown

- As the system approaches the critical point. Fluctuation diverge.
- Observable through standard deviation of the time correlation

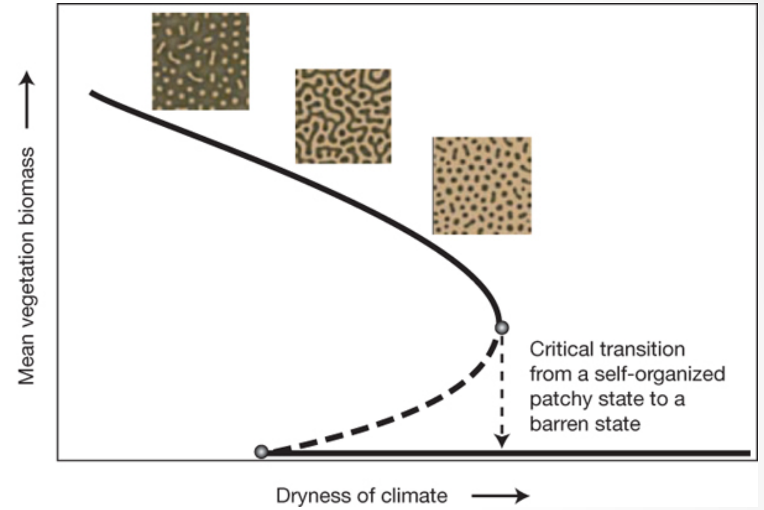
- Allows critical point detection while avoiding actual breakdown.

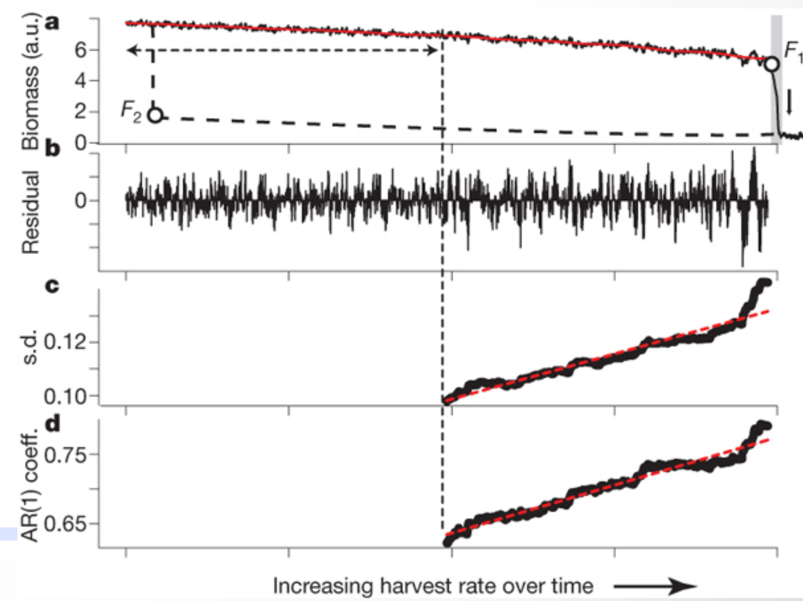
Vol 461|3 September 2009|doi:10.1038/nature08227 nature

REVIEWS

Early-warning signals for critical transitions

Marten Scheffer[1], Jordi Bascompte[2], William A. Brock[3], Victor Brovkin[5], Stephen R. Carpenter[4], Vasilis Dakos[1], Hermann Held[6], Egbert H. van Nes[1], Max Rietkerk[7] & George Sugihara[8]





Summary

- Intermittency due to collective dislocation response is well established.
  - Experimental scenarios: acoustic emission, micro-compression, image analysis.
  - Universal behavior - earth quakes, other non local bifurcating systems.
  - Analysis using phase field (non stochastic), dynamics + explicit noise, stochastic.
- Proposed a simple stochastic model to describe breakdown phenomena
  - Using a minimal model – MANY simplifying assumption – demonstrate critical behavior, bifurcation and reproduce observed BDR (E) .
  - reproduce observed Defined few experimental scenario which allow model formulation
  - Analytically (or at least numerically) solvable
- Unique experimental scenarios:
  - PDF - pre breakdown currents?
  - Pre breakdown fluctuation.
- Can serve to bridge microscopic mechanisms to experimental scenarios.
- New opportunity for stochastic analysis…