Stochastic modeling of breakdown through dislocations motion

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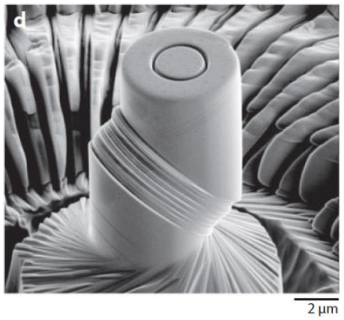
האוניברסיטה העברית בירושלים
The Hebrew University of Jerusalem

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.

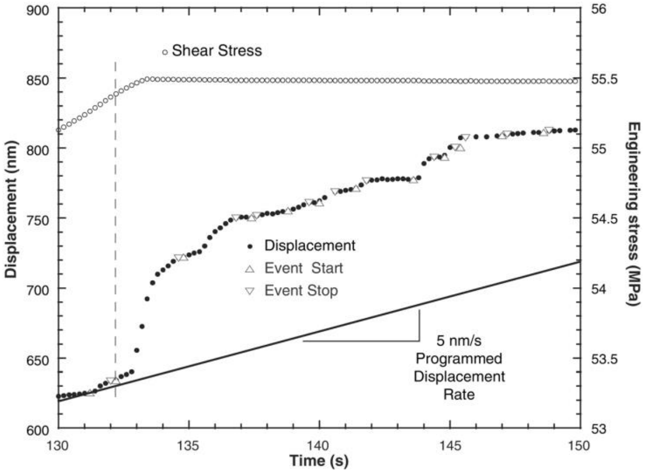
Intermittency characterized by a universal Power law burst PDF

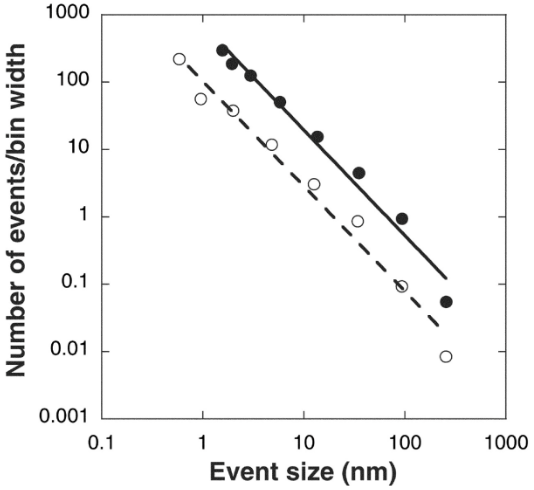
Acoustic emissions: Similar + space and time coupling between events

(Weiss & Marsan, Scjence 2003)

Earthquakes show similar PDF and spatio-temporal correlation

(Kagan, Geopgysical J. (2007)





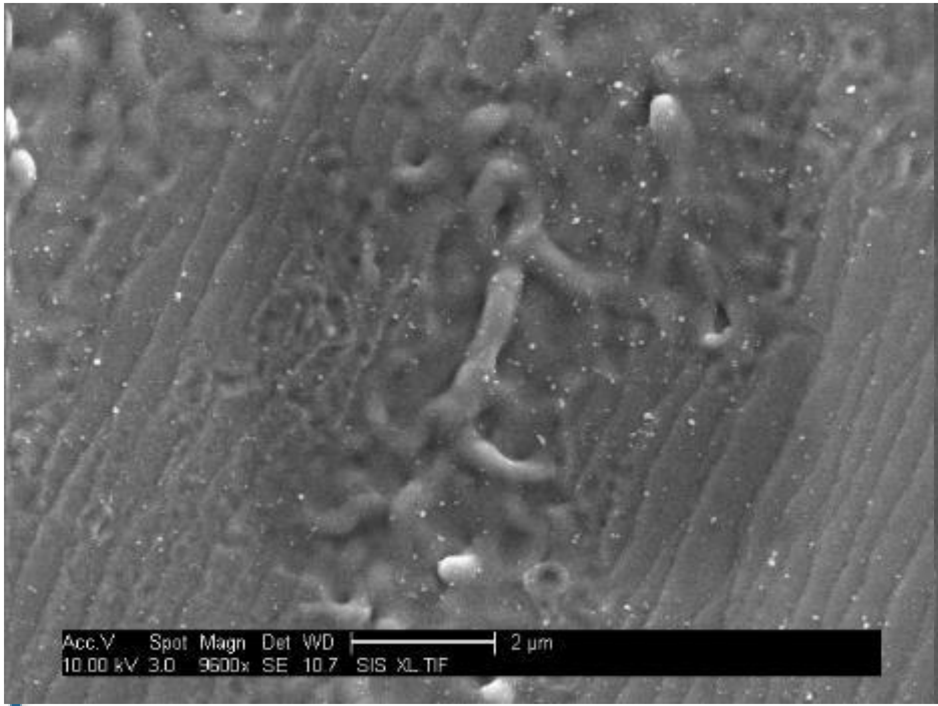
Uchic, Shade & Dimiduk, Annual Review of Materials Research (2009).

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

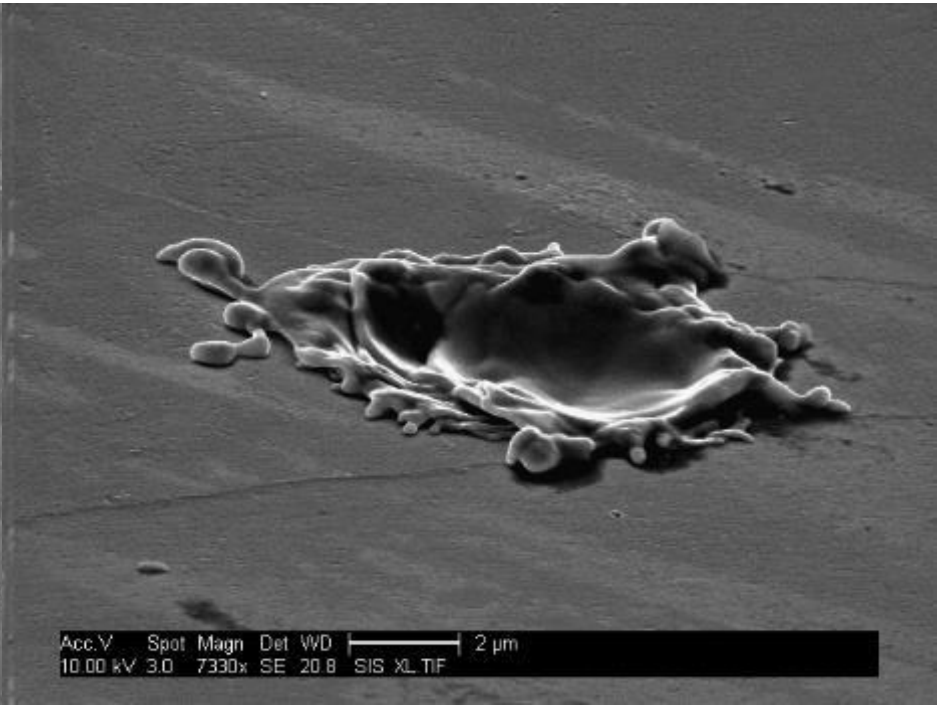
Microscopy of surface

No observable features using SEM

RF post mortem – complex deposition structures … otherwise - Flat surface.

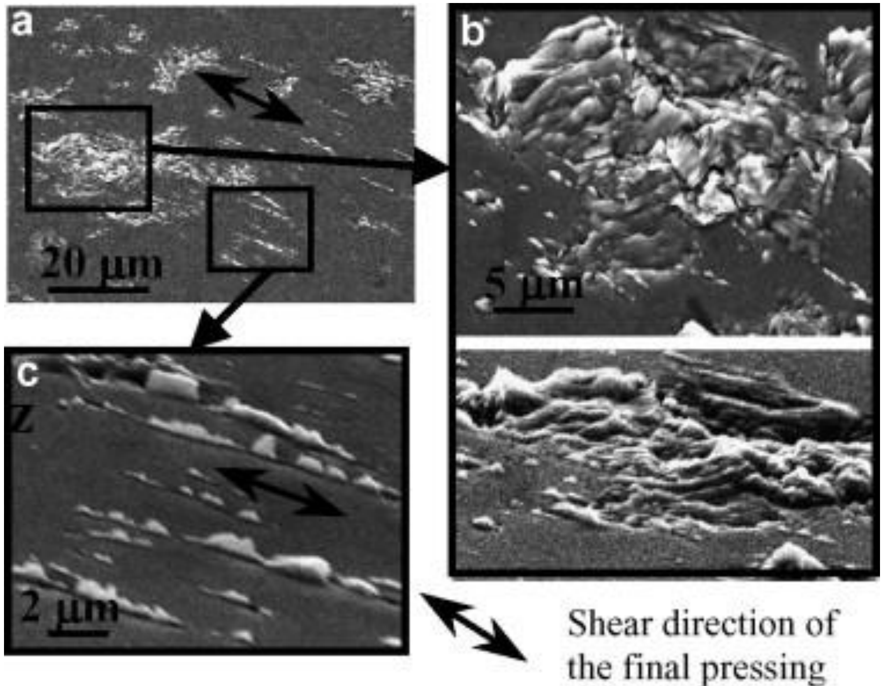


DC post mortem – aside of splashed copper … Flat surface.



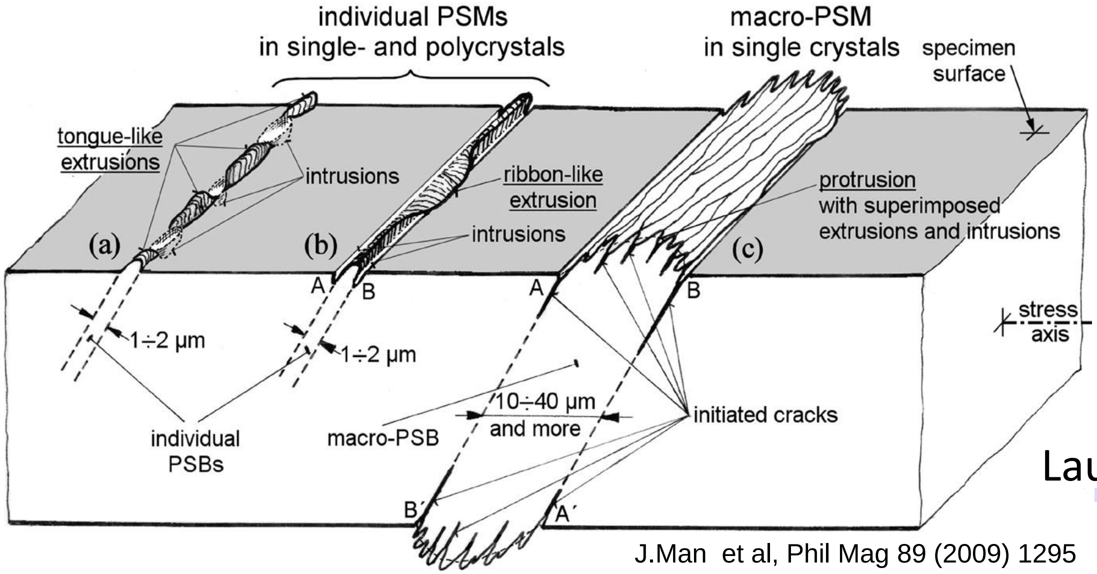
PSB -> protrusions

- Previously observed in fatigued surfaces.
- Significant sub-surface PSB leading to these surface features.

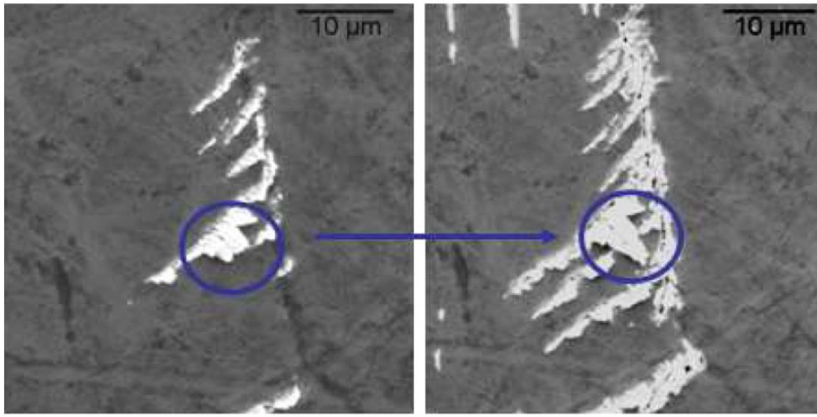


Fatigue strength and formation behavior of surface damage in ultrafine grained copper with different non-equilibrium microstructures

M. Goto et al. Int J of Fatigue. Vol 30 (2008) 1333



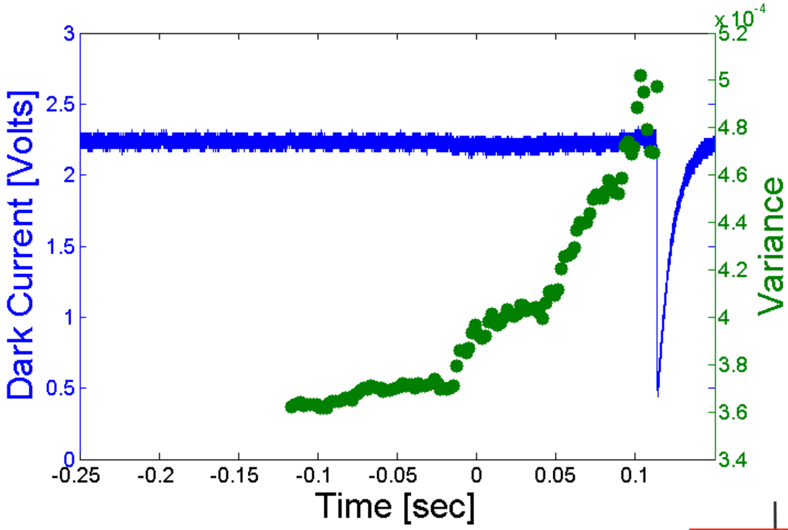
J.Man et al, Phil Mag 89 (2009) 1295

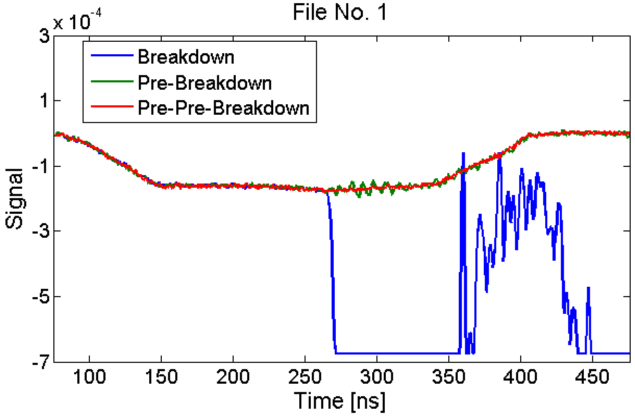


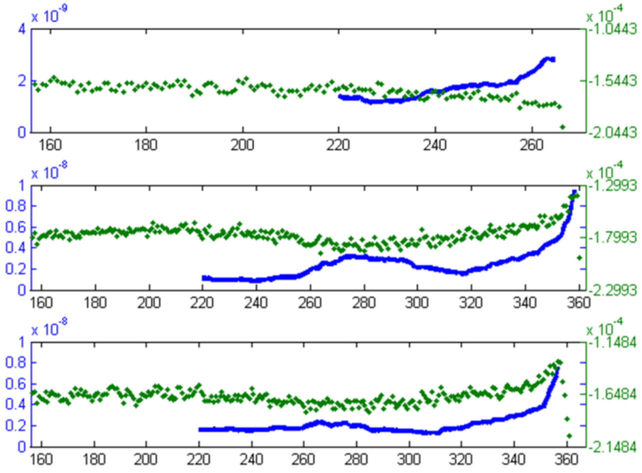
Laurent et.al. Phys Rev STAB 14 (2011) 41001

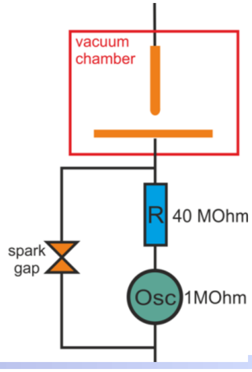
Observations until now...

- DC and RF indications of pre-breakdown increase in dark current variance









DC data –
Iaroslava Profatilova
Tomoko Muranaka

RF data - Alberto Degiovanni

What are we looking for?

- Suggest a model which will reproduce critical protrusion formation due to plastic response in the substrate?
- Criticality due to interaction between dislocations and field emitter.

Consistency with observable characteristics:

- Protrusions dynamics must allow for them to disappear:
  - No strong memory effect.
  - No observable PSB or PSM
- BD rates of similar order of magnitude as observed
- BD rate field dependency: $\mathrm{BDR} \propto E^{30} t^{5}$

Hope to achieve:

Critical experimental scenarios,

predictions of observable features (microscopy)

Possible outcomes – conditioning schemes, surface modifications, understand statistics…

0d mean field mobile dislocations model

Mean field - Single slip plane.
Define the “in-plane” mobile dislocations density (1/nm).

Protrusions forming on surface due to dislocations arriving to surface

Elastic interaction between dislocations

Field enhancement due to protrusion leads to increase in localized stress

Simulating up to creation of a runaway process which will lead to eventual tip evaporation

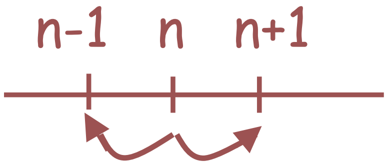
Not yet in…
Surface evolution – leads to hardening due to cellular structure interaction between sites

General gain-loss type Markovian processes

Rates for transition between states

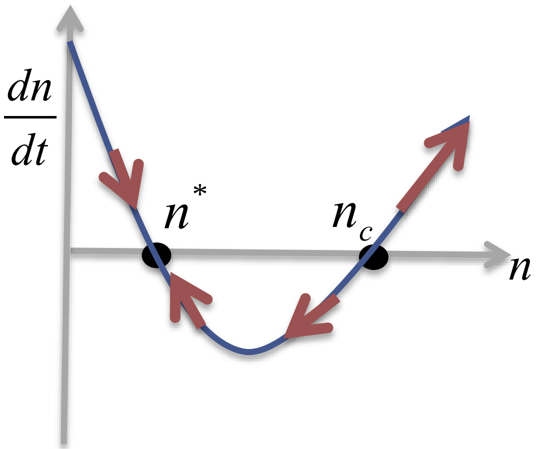
$$n \xrightarrow{\rho_n^+} n+1$$

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



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)

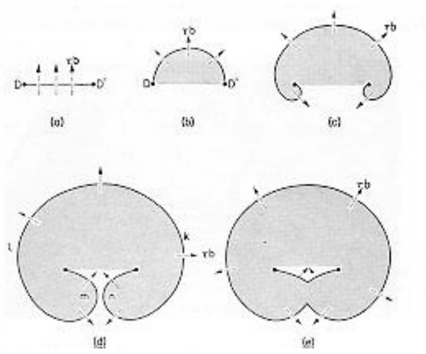
Approximate solution based on WKB theory with 1/N being the small parameter.

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

Assaf and Meerson, PRE 2010

Moving dislocations population

- Classical multiplication through frank-reed sources



- Multiplication rate:

○Activation of existing FR sources.

$$\frac{d\rho^{+}}{dt} = \alpha \frac{\rho + c}{t_{\text{create}}} P_f$$

○Creation time calculated using dislocation velocity and stress dependent FR source size

$$\sigma = \frac{2Gb}{L}$$

○Activation requires overcoming local obstacles -

$$\left(c_{v(T)} + \rho + c\right) e^{\frac{\Omega\sigma}{k_B T}}$$

Final term includes a dimensionless
Kinetic factor

$$\frac{d\rho^{+}}{dt} = \frac{\kappa v}{2Gb} (\rho + c)^{2} \sigma e^{\frac{\Omega\sigma}{k_B T}}$$

Moving dislocations population

- Depletion rate
  - Collisions with obstacles
  - Collisions with other moving dislocations
  - Ejection to surface
  - Add an interaction factor (not all dislocations are removed due to thee interactions)

$$\frac{d\rho^-}{dt} = \rho c v + \rho^2 v + \delta \frac{\rho}{t_{\text{life}}}$$

$$\frac{d\rho^-}{dt} = \xi v \left(\rho + c + \frac{\delta}{D}\right) \rho$$

- State variables:
  - Velocity proportional to stress
  - Stress – Maxwell + stress due to elastic interaction between dislocations
  - Field enhancement

$$\begin{aligned} v &= 50 C_t \frac{\sigma}{G} \\ \sigma &= B \frac{1}{2} \varepsilon_0 E^2 + Z G b \rho \\ E &= \frac{V}{d} (\beta + 3.5) \end{aligned}$$

Protrusions and field interaction

- Using number of new steps

$$N = \int \dot{N} dt = \int vC\rho dt$$

- Define local change in aspect ratio

$$\frac{d\beta^{+}}{dt} = 2N\dot{N} = 2\sqrt{\beta}vC\rho$$

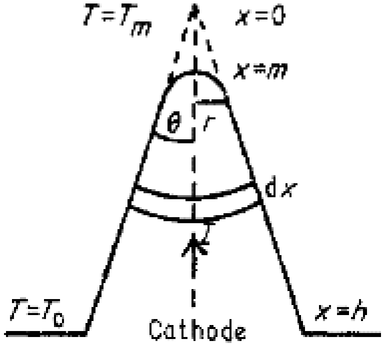
- Decay through surface diffusion

$$\frac{d\beta^{-}}{dt} = \eta B_d \beta \qquad B_d = \frac{D_{s0} e^{-\frac{Q}{k_B T_{\mathrm{tip}}}} \gamma \Omega^2 \nu}{k_B T_{\mathrm{tip}} l^4}$$

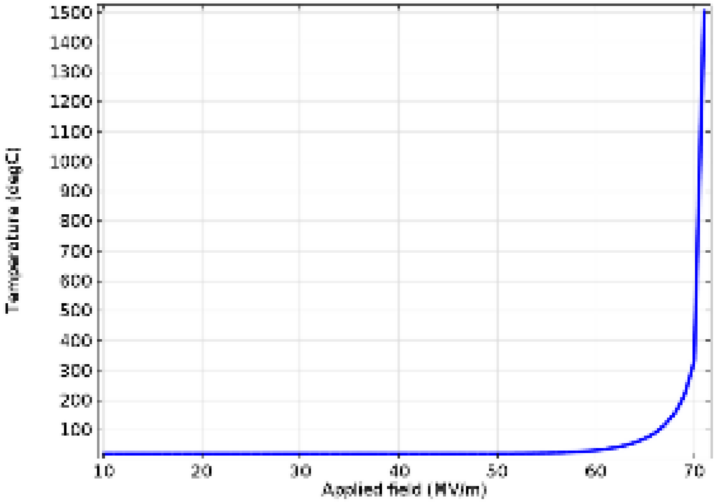
- Beta used to enhance local field and control FN current

Temperature effect on dynamics of protrusions

- Stresses:
  - Heat conduction leads to negligible temperature change at the base of the protrusion and therefor negligible thermal stresses.
- Surface relaxation
  - Temperature estimated at the tip close to BD is very high (> 1000K)
  - activation energy for surface relaxation is very low 0.03eV, Therefor diffusion is fast and changes are up to factor of 2 once a tip is formed.



Analytic calculations by Sergio calatroni



Numerical simulations by Vahur Zadin

Linear Stability Analysis for estimating fast dynamics reduced form

- Linearization of the full model:

$$\begin{pmatrix} \dot{\Delta\rho} \\ \dot{\Delta\beta} \end{pmatrix} = \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} \begin{pmatrix} \Delta\rho \\ \Delta\beta \end{pmatrix}$$

- The eigenvalues and eigenvectors indicates the change rates and the dynamic dependencies of the variables.
- For the basic eigenvectors, each variable dynamics is independent:

$$\begin{pmatrix} \dot{\Delta\rho} \\ \dot{\Delta\beta} \end{pmatrix} = \begin{pmatrix} \lambda_\rho \Delta\rho \\ \lambda_\beta \Delta\beta \end{pmatrix} \Longrightarrow \begin{pmatrix} \Delta\rho \\ \Delta\beta \end{pmatrix} \propto \begin{pmatrix} e^{\lambda_\rho t} \\ e^{\lambda_\beta t} \end{pmatrix}$$

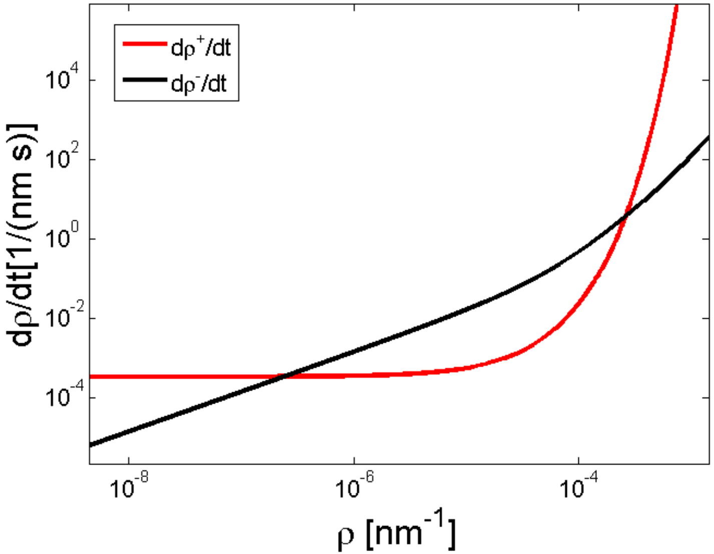
$$\begin{aligned} A_{1,1} &= \frac{25\kappa C_t}{G^2 b} e^{\frac{\Omega\sigma_*}{k_B T}} (\rho_* + c) \left[2\sigma_*^2 + ZGb(\rho_* + c) \left[2ZGb\rho_* + B\varepsilon_0 E_0^2 (\beta_* + 3.5)^2 + \frac{\Omega\sigma_*^2}{k_B T} \right] \right] \\ &- \frac{50\xi C_t}{G} \left[\sigma_* \left(2\rho_* + c + \frac{\delta}{D} \right) + ZGb\rho_* \left(\rho_* + c + \frac{\delta}{D} \right) \right] \\ A_{1,2} &= \frac{25\kappa C_t}{G^2 b} e^{\frac{\Omega\sigma_*}{k_B T}} B\varepsilon_0 E_0^2 (\rho_* + c)^2 (\beta_* + \\ &- \frac{50\xi C_t}{G} \rho_* \left(\rho_* + c + \frac{\delta}{D} \right) B\varepsilon_0 E_0^2 (\\ A_{2,1} &= \frac{100 C_t C}{G} \sqrt{\beta_*} (\sigma_* + ZGb\rho_*) \\ A_{2,2} &= \frac{100 C_t C}{G} \left[\sqrt{\beta_*} \rho_* B\varepsilon_0 E_0^2 (\beta_* + 3.5) + \sigma_* \frac{\rho_*}{2 sqrt \beta_*} - \eta B_d \right] \end{aligned}$$

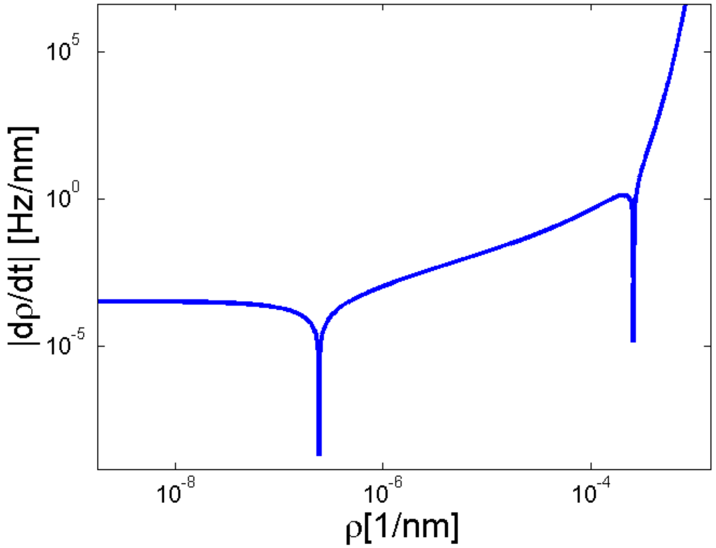
- For strong diffusion we get this situation and beta rates are significantly smaller than rho.

Reduced – single dynamics model

- Strong surface relaxation lead to surface protrusions following instantaneously the dislocation population.

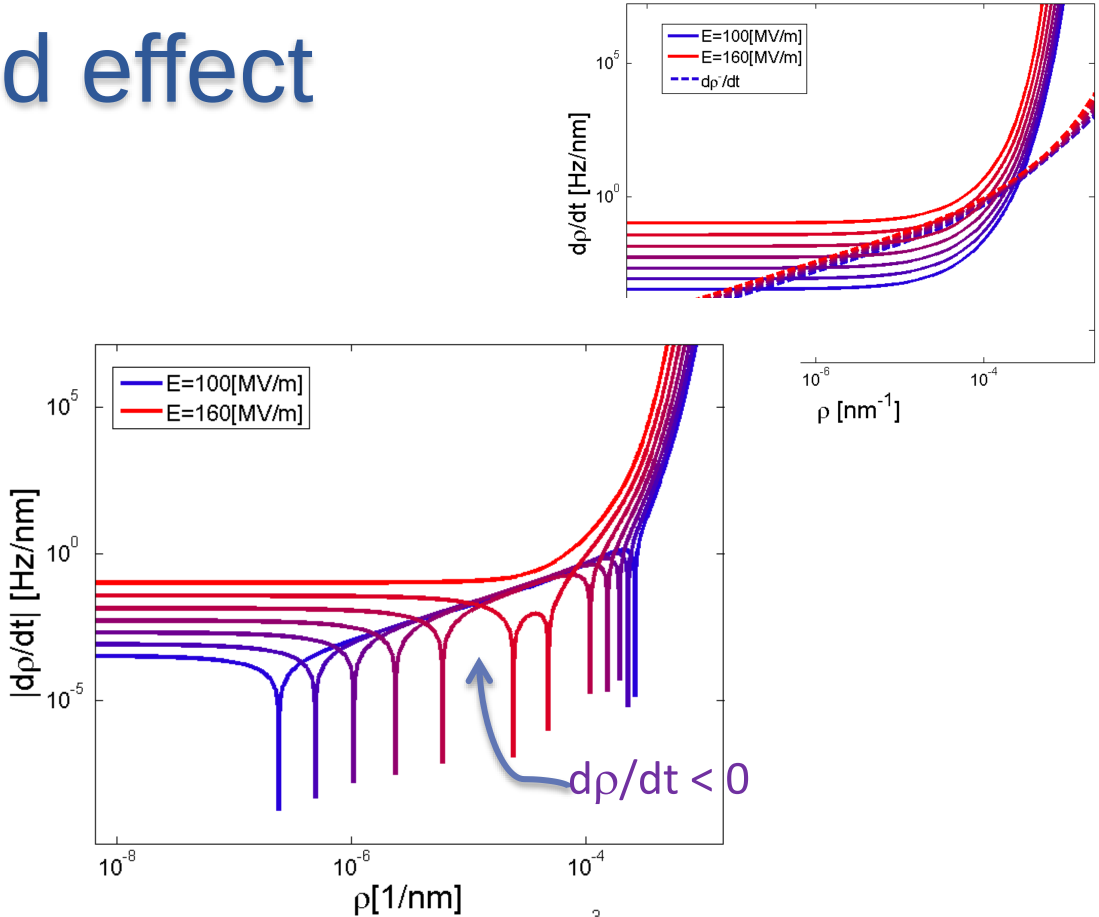
  Protrusion height is now given by $\beta = E_s \rho^2$
- The model is characterized by two points:
  - ○ Metastable
  - ○ a critical point





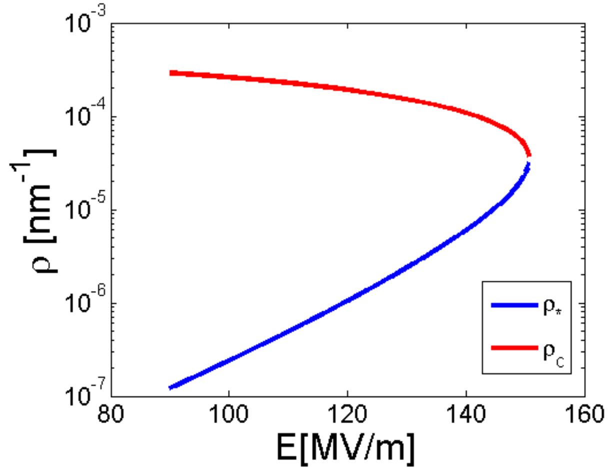
Applied field effect

Low fields:
Mobile dislocation density remains at Metastable region.
Dynamic barrier decreases with increasing fields.



dρ/dt < 0

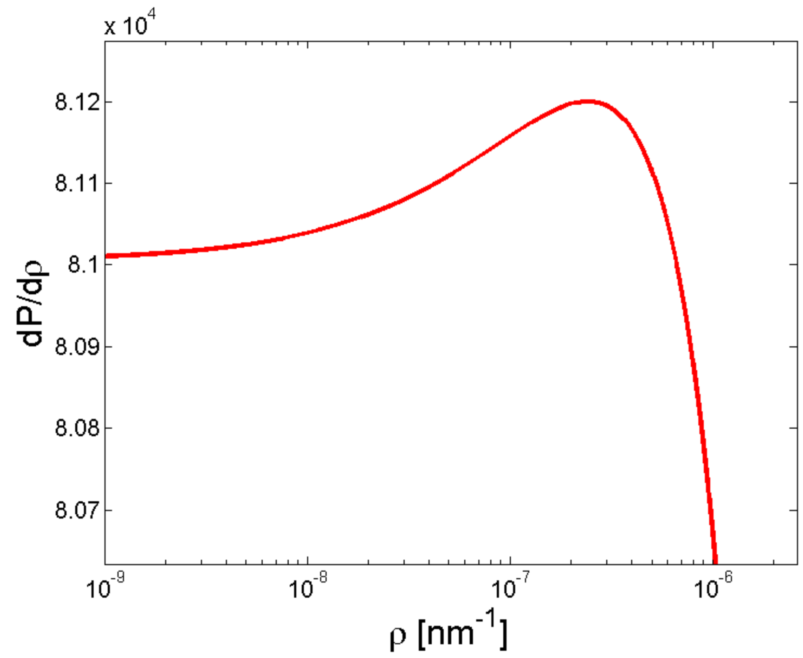
Up to a critical stress – bifurcation to two solutions.
Above it - no meta-stable state solution.

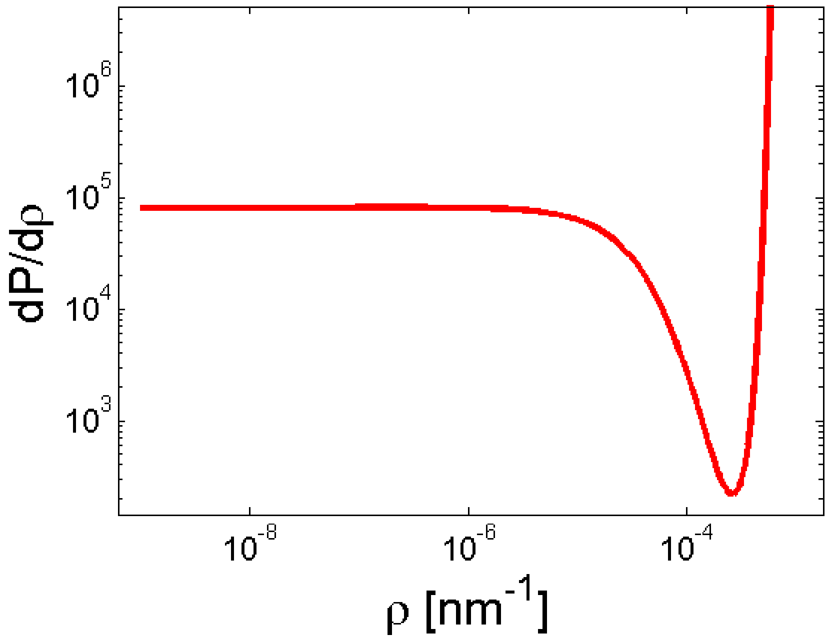


PDF of dislocation population

The single parameter model can be solved analytically to give the Probability density function of the dislocation density

This indeed shows a low metastable solution and a probability barrier formation



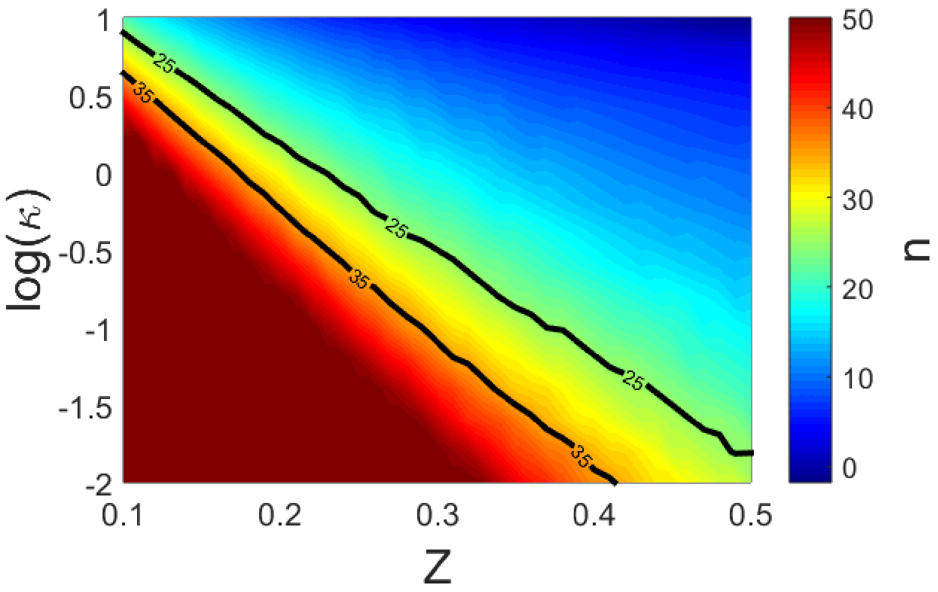


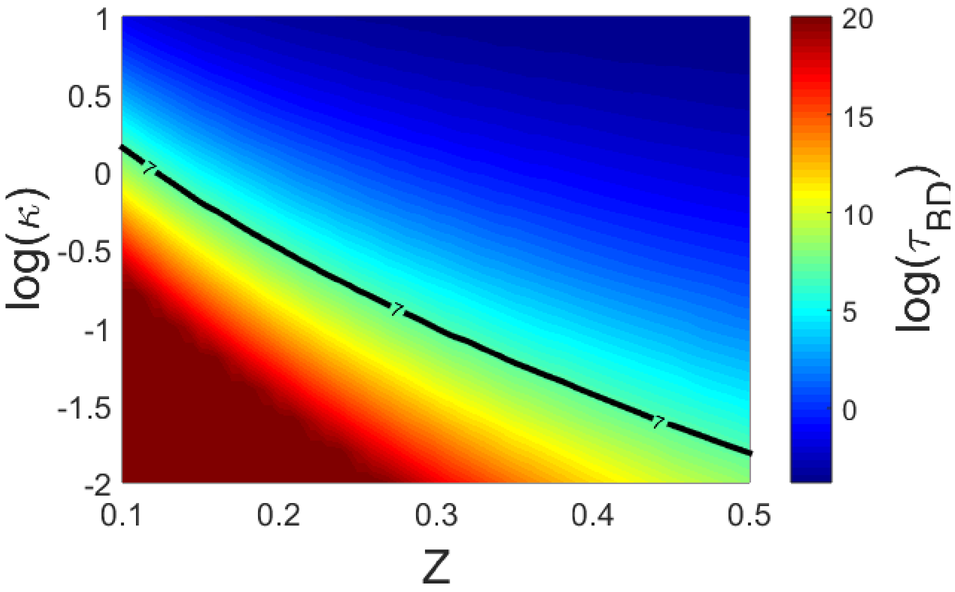
Parametrization

- The model contains various competing mechanisms which can not be readily estimated.
- We scan the parameter space to see if a combination of such parameters does allow for observable behavior
- If such a region in parameter space does exist we can then check whether such a combination is indeed physically viable.

- Two main observables are used for that
- Experimental BD rates: 10^{-7} [bpp/m]
  - Estimating the number of active regions per m :
    $$N\left(\frac{1}{m}\right) = \frac{(\frac{N_{iris}}{m})\cdot(S_{iris})}{dR_{active\ regions}{}^{2}} \approx \frac{100\cdot 2\pi\cdot 2.35(mm)\cdot 1(mm)}{(10^{-2}mm)^{2}} = 10^{7}$$
  - Since the pulses are of 230 nsec we get :
    $$\tau(BD)_{per\ area\ unit} = dt_p/(P(bpp/m)/N) = \frac{230nsec}{\frac{10^{-7}}{10^{7}}} \approx 10^{7}\left(\frac{sec}{zone}\right)$$
- Field dependency of the breakdown rate (estimated as E^{30}) .
  So we define the localized (10%) exponent : $n = \log_{1.1}\left(\frac{\tau(E)}{\tau(1.1\cdot E)}\right) \approx 30$

Parameter space –analytic model





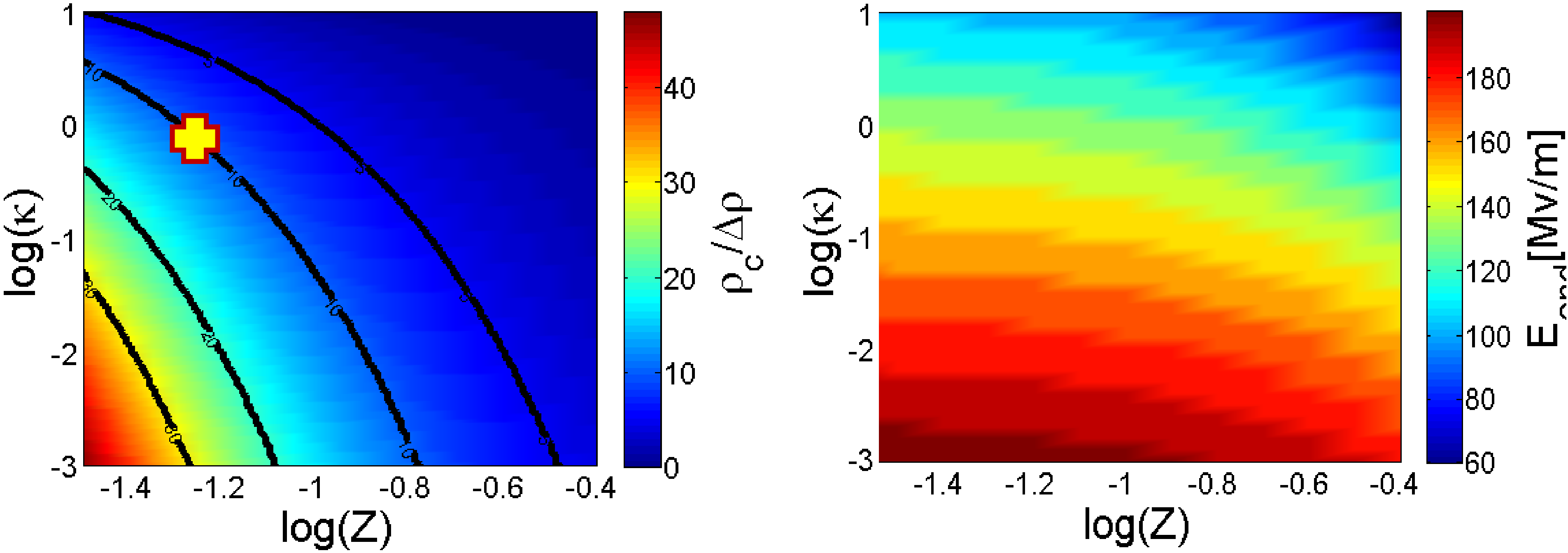
- Observable values:

$$\tau_{bd} \approx 10^7 sec\ , n = ln(\frac{\tau(E)}{\tau(rE)})/\ln(r) \approx 30$$

- Significant coincidence region:

Parameter space – kmc simulations

- full model validity range – using kmc

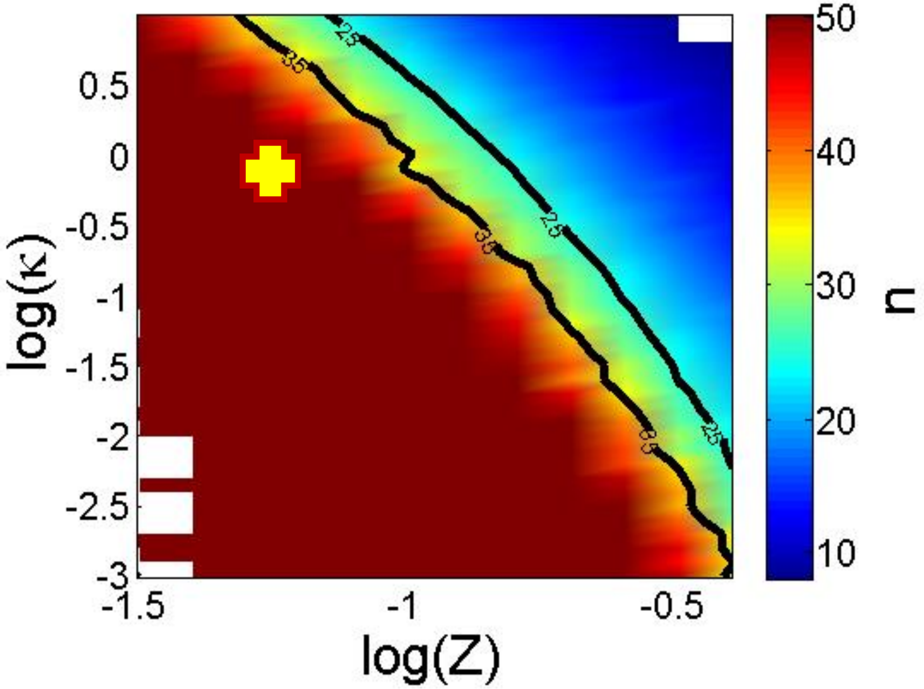


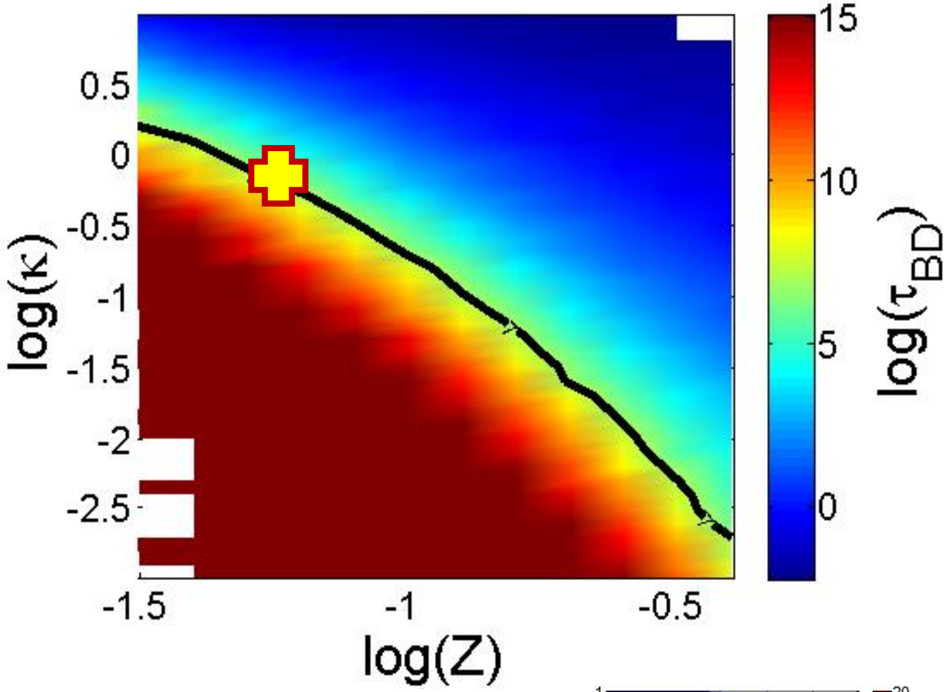
Arbitrarily choose example working point :

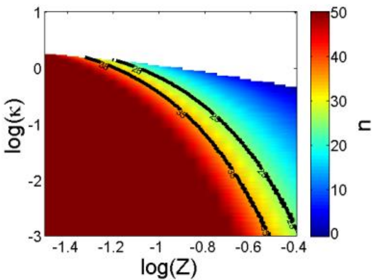
maximal field
kmc accessible

Parameter space – kmc simulations

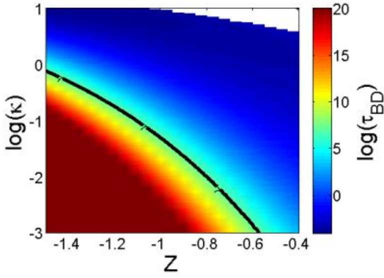
- full model validity range – using kmc

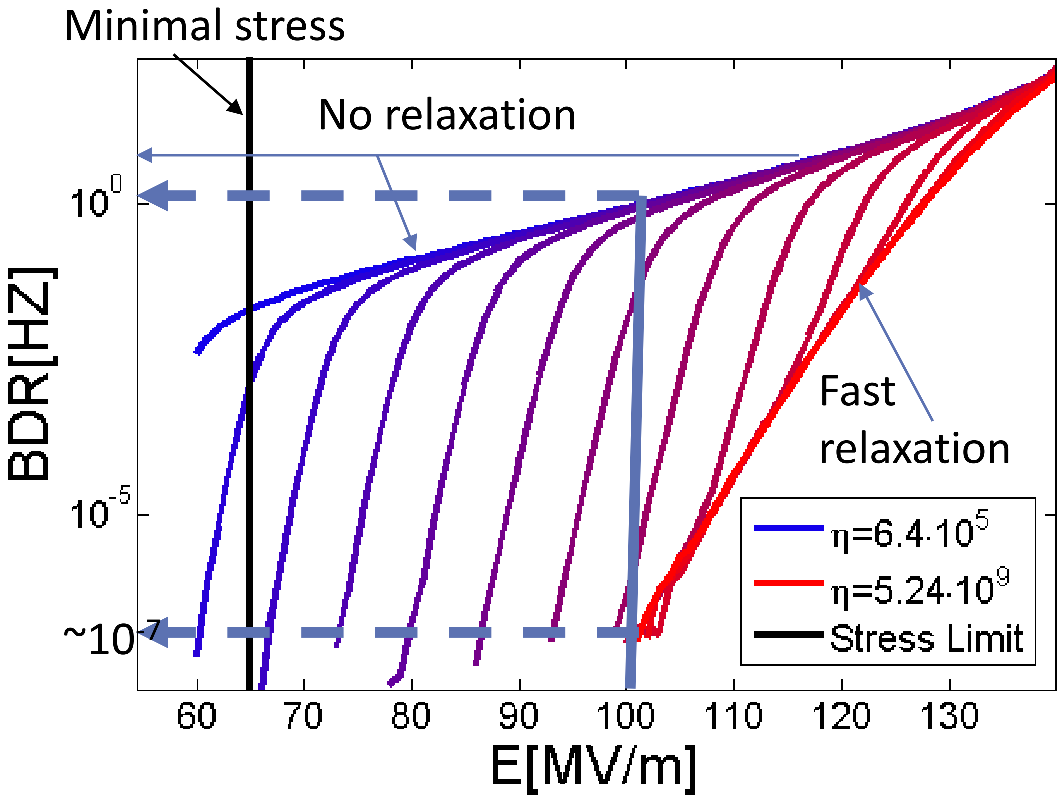






Need for further model calibration…..



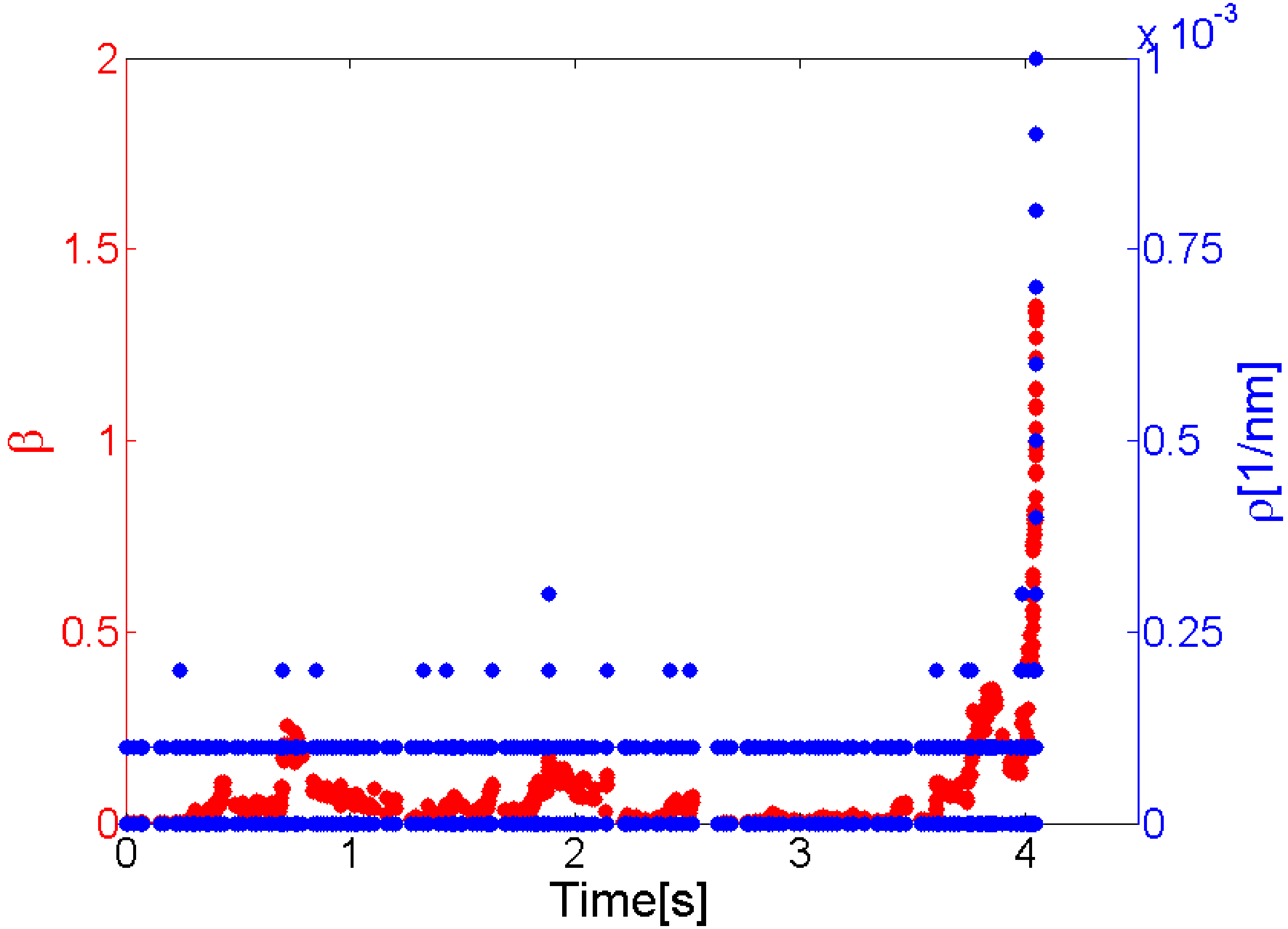


Relaxation kinetics (surface diffusion) defines two limits:

a. Fast- surface topography follows mobile dislocations content.
b. Slow- surface builds up even at metastable state of mobile dislocations .

Evolution trajectories

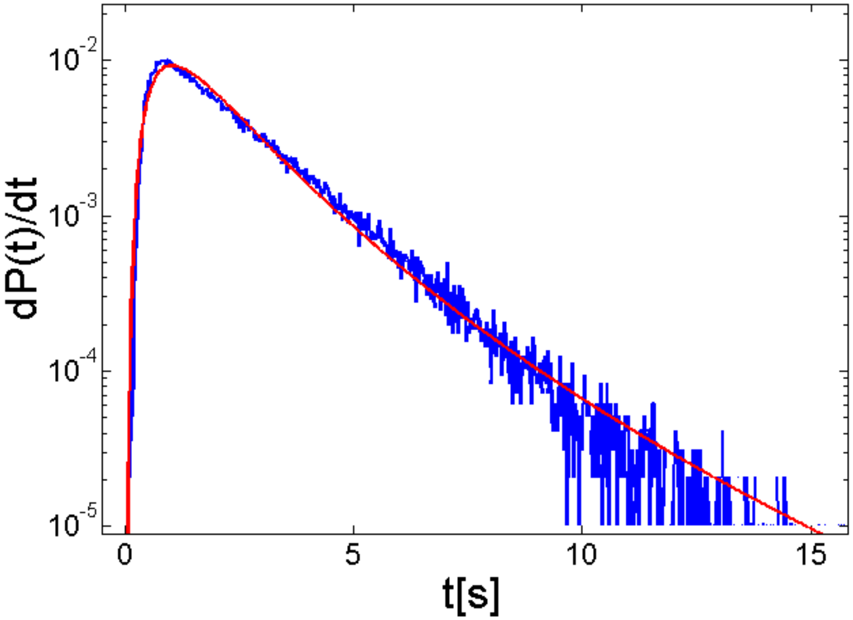
- Dynamics of surface protrusions shows relation between surface protrusions and mobile dislocations.



Implication to BD time distributions

The interaction between
Surface protrusion evolution
And mobile dislocation content
Leads to a non-Poissonian distribution

This implies a strong dependence
Of BD rate on pulse length.



Histogram of time to BD shows a log normal behavior for κ=0.05, Z=0.6.

$$f_X(x;\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}}\ \exp\left(-\frac{(\ln x-\mu)^2}{2\sigma^2}\right)$$

σ = 0.7[log(s)], μ = 0.5[log(s)]

Signs of criticality

- Adiabatically moving between quasi-stationary PDF:
  Change in pdf moments with field

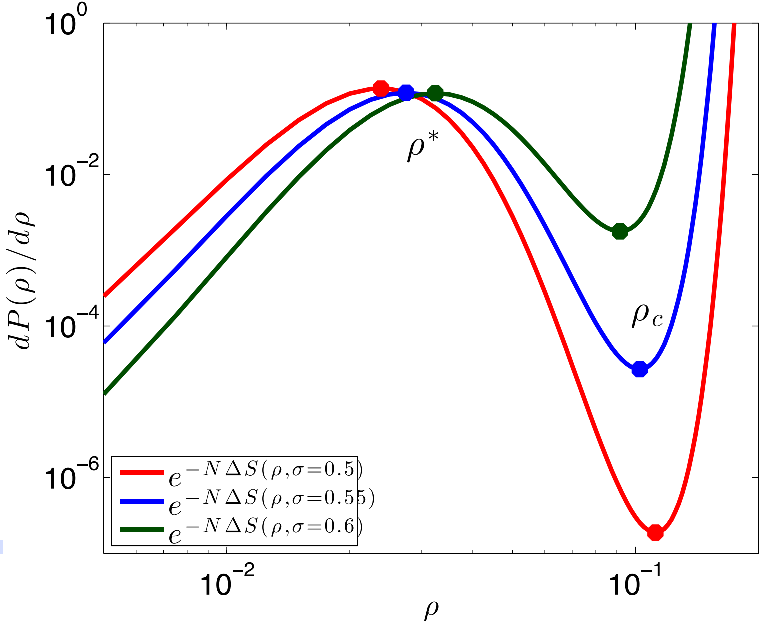
  -> identify threshold

- At specific conditions, probe time dependencies of the QS pdf:
  Identify large fluctuations time dependency

  -> identify time constants

  -> mechanism

$$P_c(s,r,t)=\int_0^t P(s,r'>r,t')dt'$$



PRE-BD signals

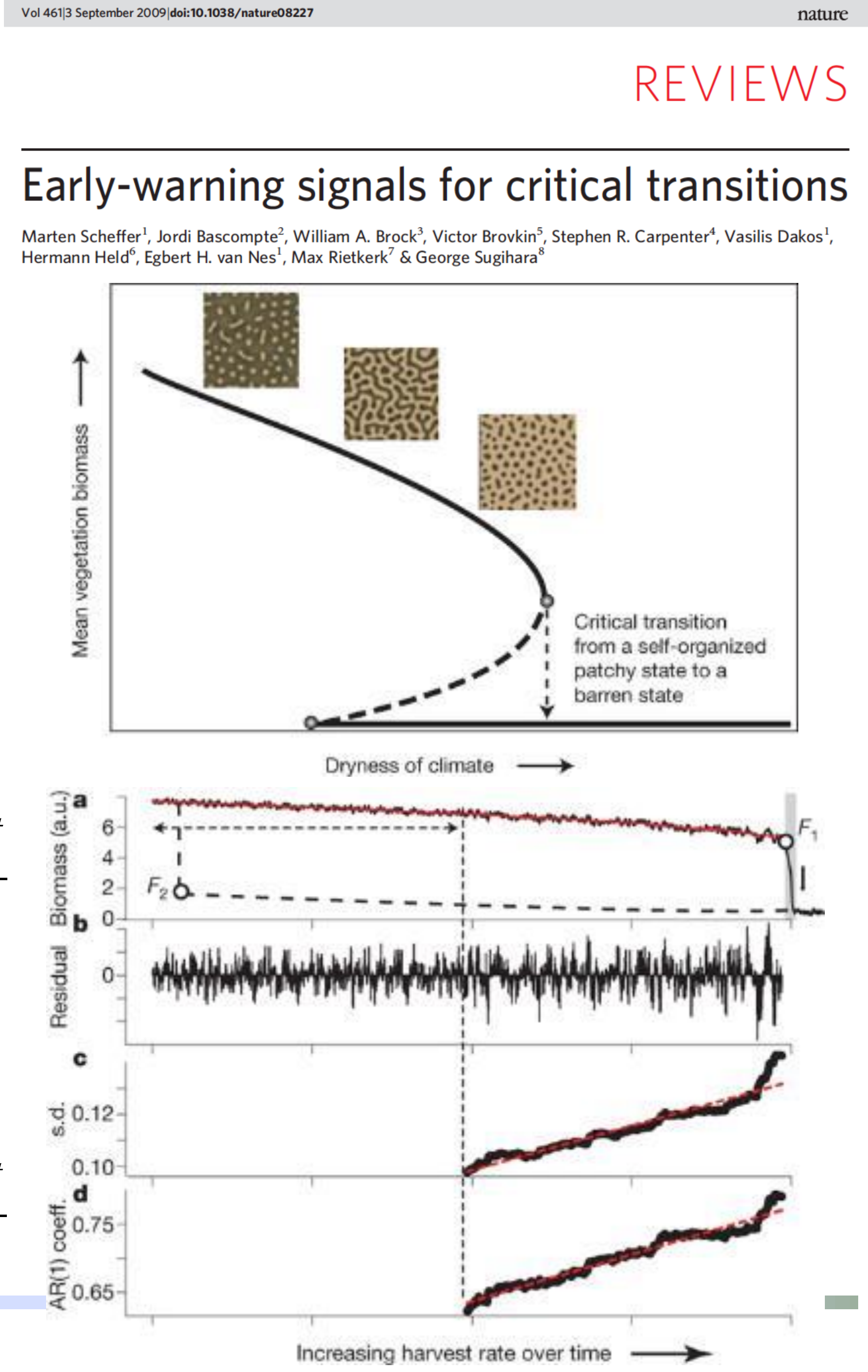
- As the system approaches the critical point. Fluctuation diverge.
- Observable through standard deviation of the time correlation

$$SD(t) = \frac{\int_{t-D}^{t+D} \left(I(t) - <I>\right)^2 dt}{\left(<I>\right)^2}$$

- Or, more generally, autocorrelation in the signal

$$R(k) = \frac{\int_0^{t-k} \left(I(t) - <I>\right)\left(I(t+k) - <I>\right) dt}{\int_0^{t-k} \left(I(t) - <I>\right)^2 dt}$$

-



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

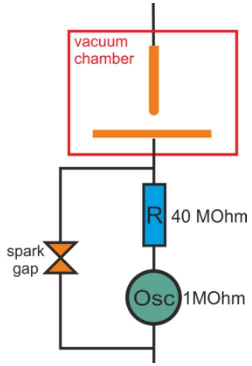
nature

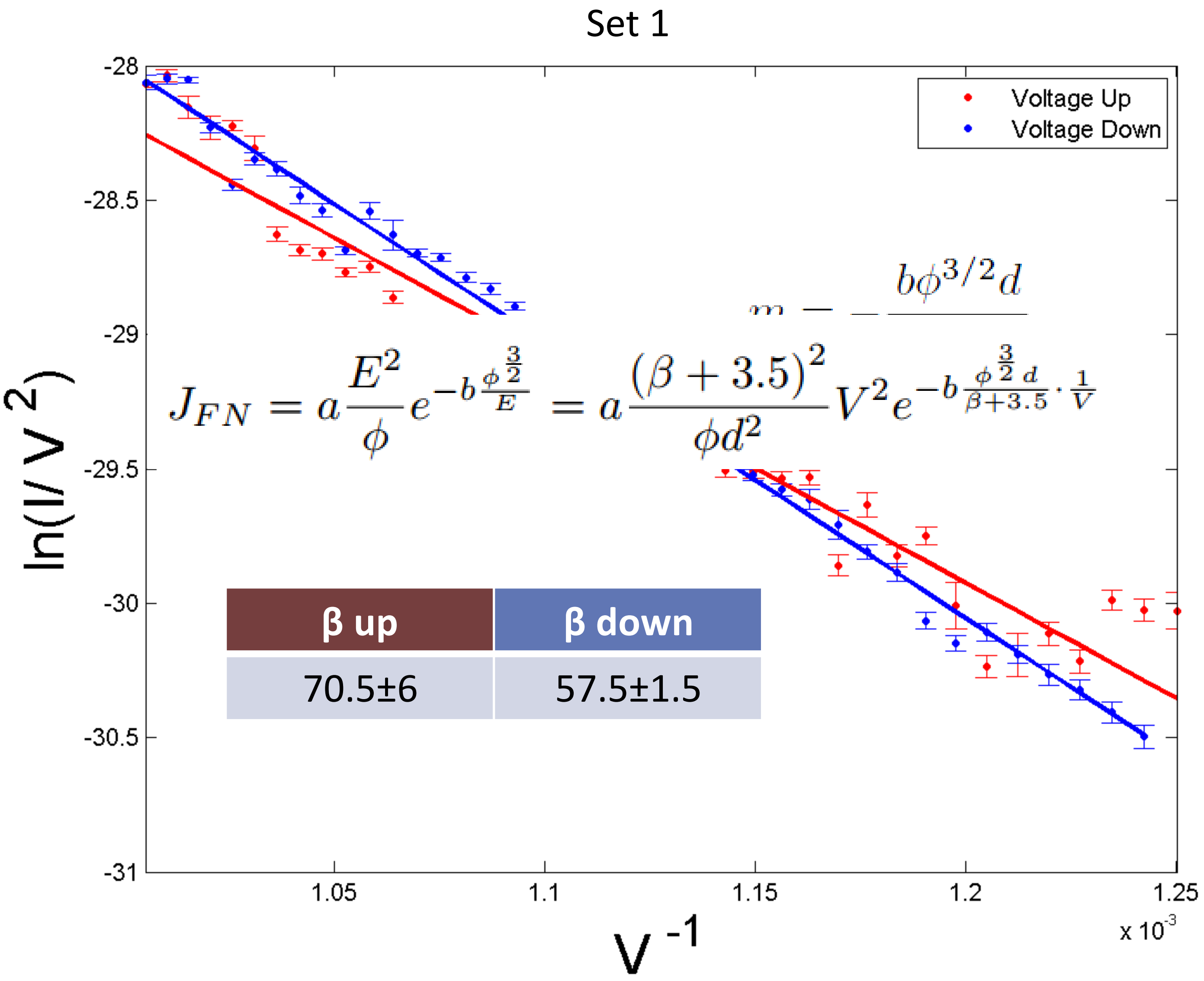
REVIEWS

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]

DC measurements





$$m = -\frac{b\phi^{3/2}d}{}$$

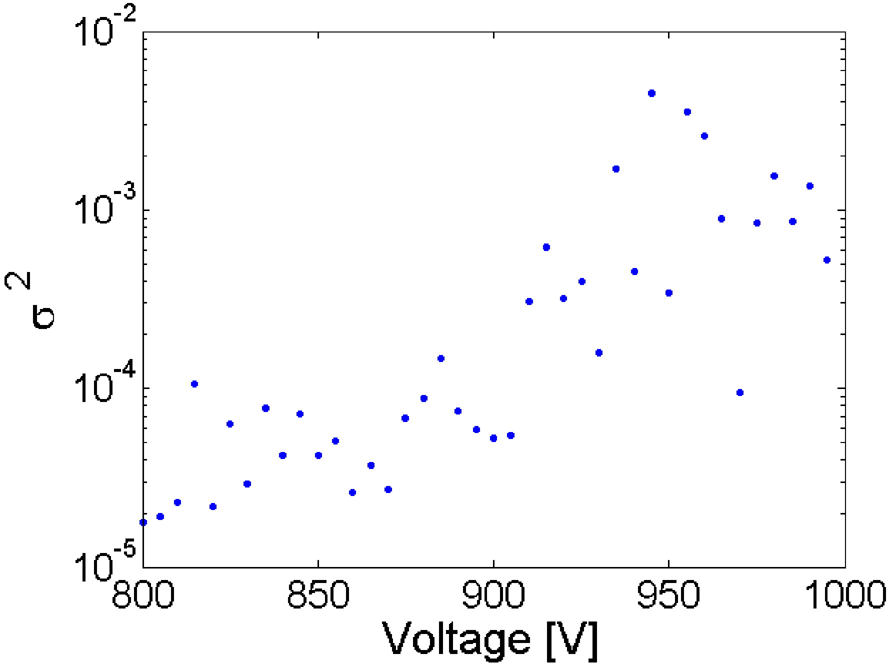
$$J_{FN} = a\frac{E^2}{\phi}e^{-b\frac{\phi^{\frac{3}{2}}}{E}} = a\frac{(\beta+3.5)^2}{\phi d^2}V^2 e^{-b\frac{\phi^{\frac{3}{2}}d}{\beta+3.5}\cdot\frac{1}{V}}$$

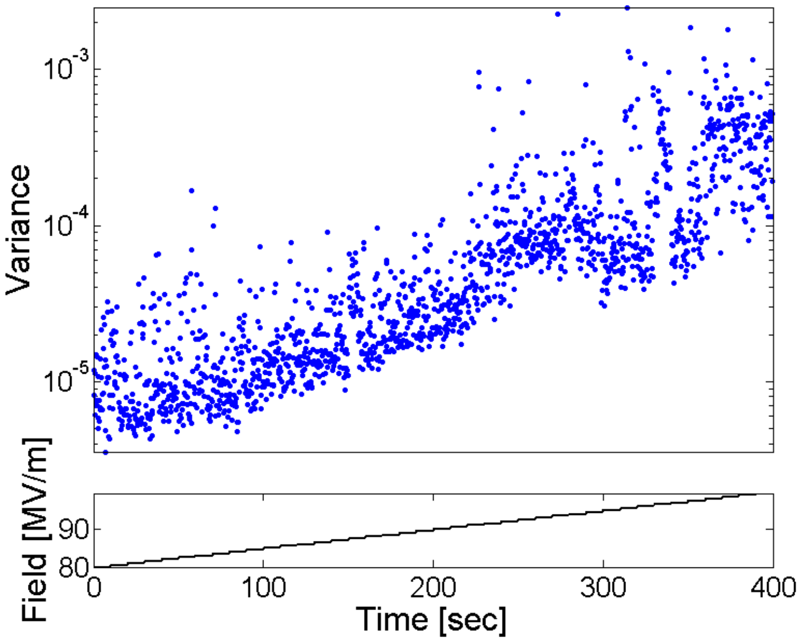
β up	β down
70.5±6	57.5±1.5

Tomoko Muranaka, Robin

Field dependent fluctuations

- Monitoring FN allows direct access to the protrusion population, and therefor show pre BD increase.
- Time scale of fluctuations - indicative to the dynamic timescale.





Summary

- BD due to critical plastic process.
  - demonstrate critical behavior, bifurcation order of magnitude effect.
  - Analytically (or at least numerically) solvable
  - reproduce observed BDR exponent
- Unique experimental scenarios:
  - PDF - pre breakdown analysis: using PDF (fluctuations) and PDF tail (rare events).
- Future directions
  - Better dark current measurements.
  - Full fit of the model.
  - Predict acoustic signal.
- Possible Implications - conditioning through surface hardening (enriching forest dislocations), effect of surface and microstructure.
- Possible observations - Cellular structure observable via TEM? SEM? Acoustic signal?

- Fitted values (kinetic factors etc) should be compared to microscopic models.