Stochastic modelling of BD nucleation

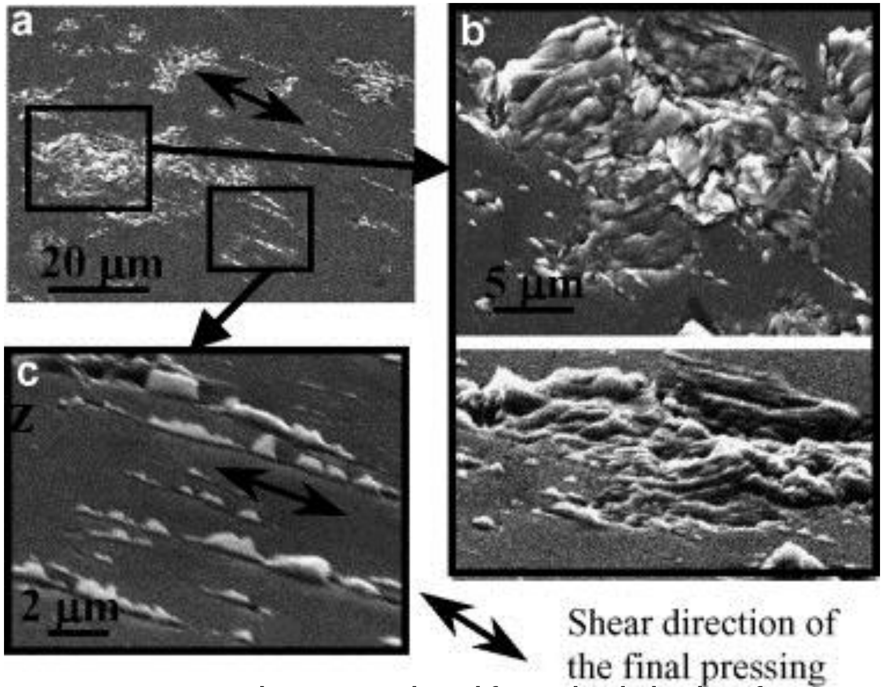
Amit Weiss, Eli Engelberg
, Yinon Ashkenazy

Racah Institute of Physics,

Hebrew University, Jerusalem, Israel

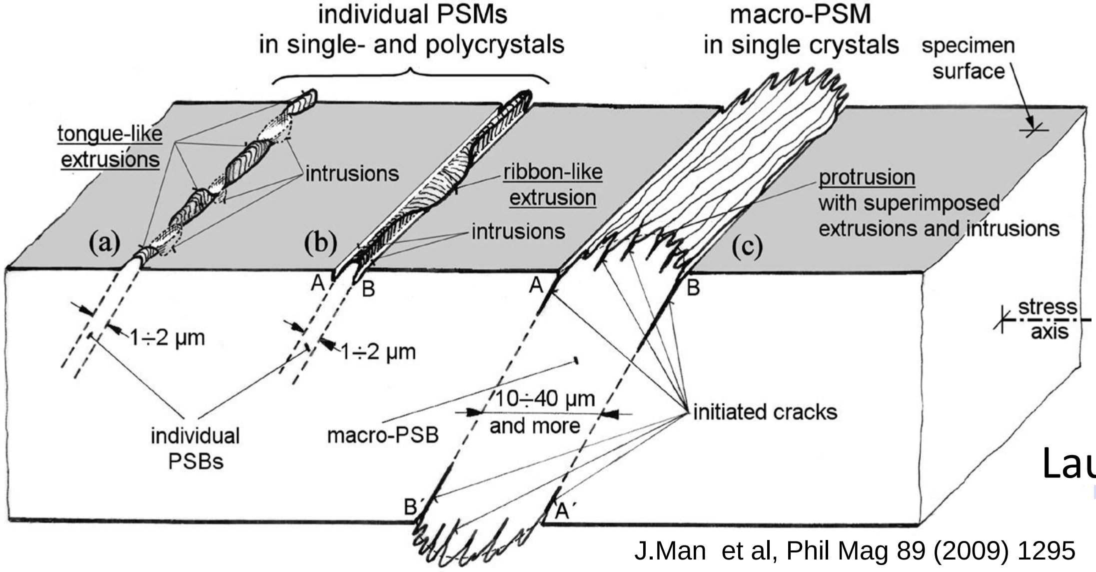
PSB -> protrusions

- Previously observed in fatigued surfaces.
- Significant sub-surface PSB leading to these surface features.
- Stochastic response at sub-yield stresses.

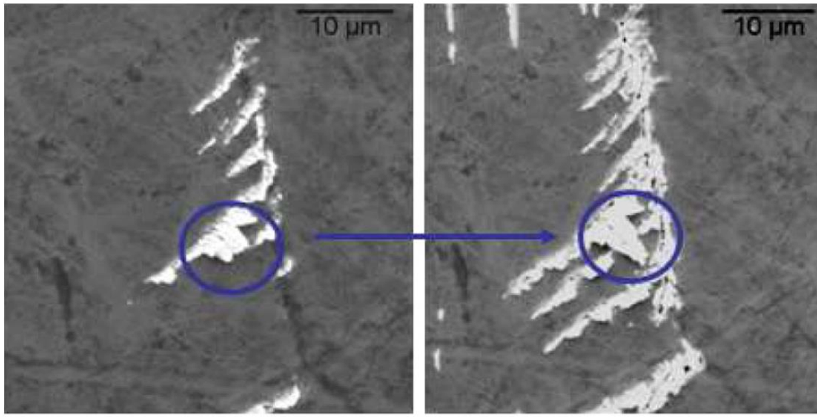


Fatigue strength and formation behavior of surface damage in ultrafine grained copper with different non-equilibrium microstructures

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

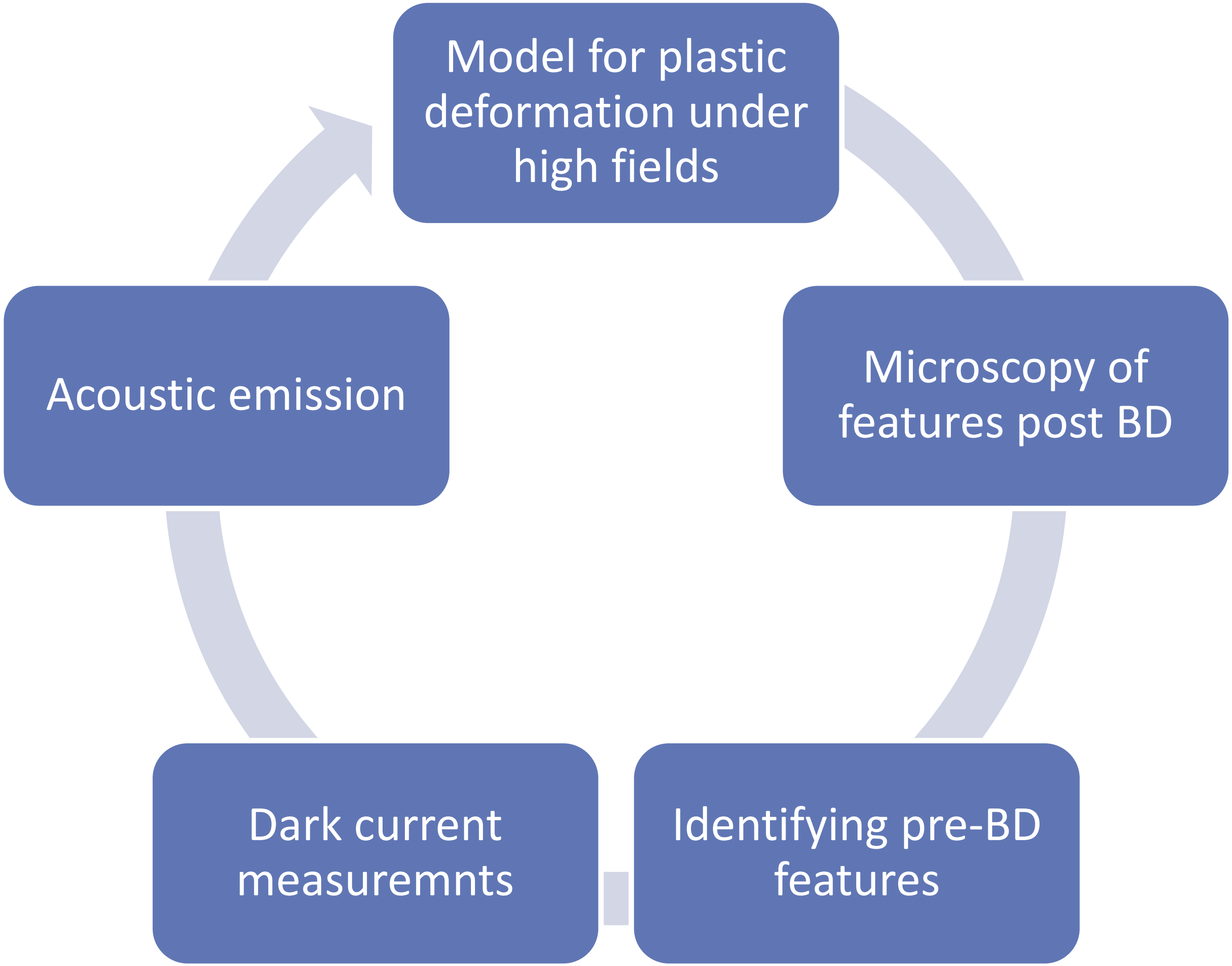


J.Man et al, Phil Mag 89 (2009) 1295



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

Trying to validate and calibrate a model



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

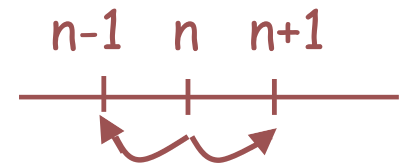
Not yet in…
Surface evolution – leads to hardening due to cellular structure interaction between sites

General gain-loss type Markovian processes

Rates for transition between states

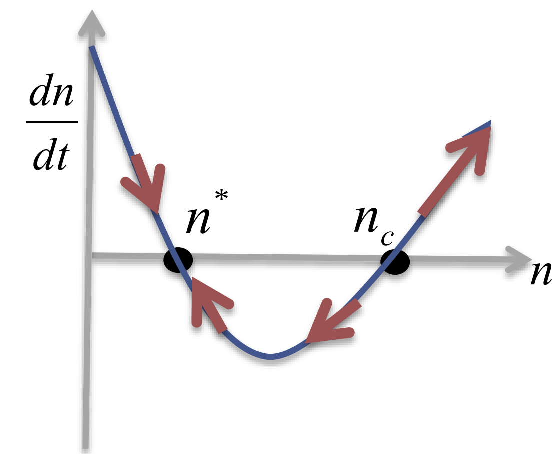
$$n \xrightarrow{\rho_n^+} n+1$$

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



The master equation

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



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.

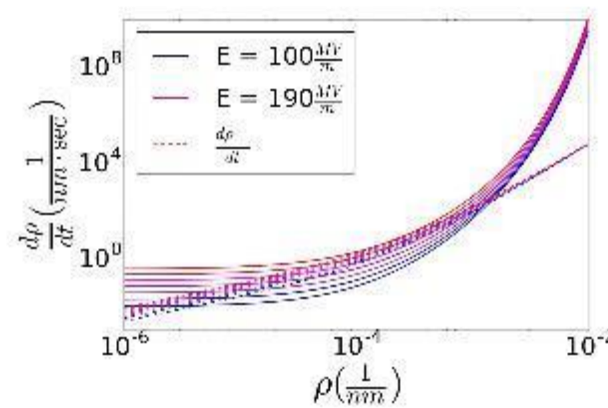
$$\dot{P} = 0 \quad \Rightarrow \quad P(n) \equiv P(r N) \sim e^{-N[S(r)+O(1/N)]}$$

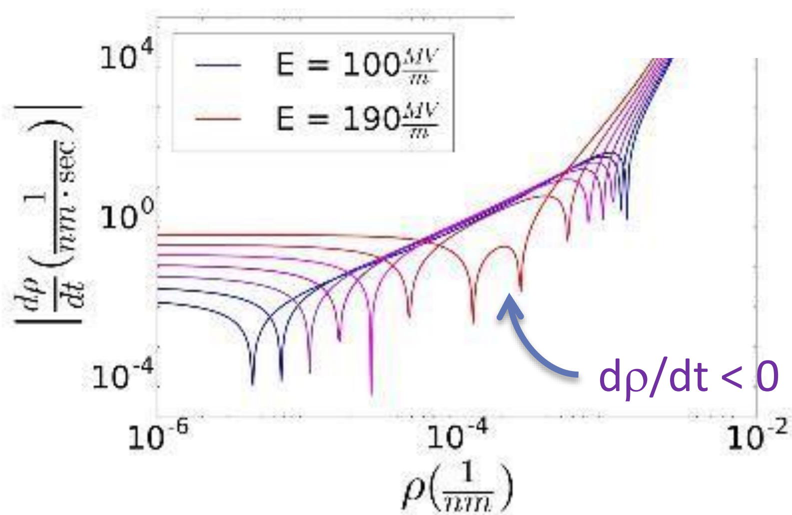
Model basics

- Mobile dislocation multiply:
  - Activate sources
  - Release sessile dislocations at pile-ups
  - Protrusion effect on stress and temperature
- Mobile dislocations depletion
  - Collision - obstacles, other moving dislcaoitns, surface
- Protrusion form due to accumulation of dislocations but relax through diffusion (a kinetic factor)
- The problem – multi physics + multi parameters
  - First trials – use what we have
  - Better trials- learn what we need

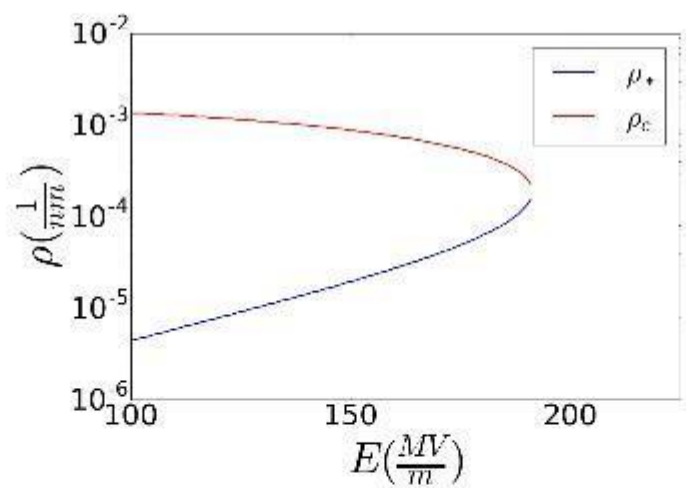
Applied field effect

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





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

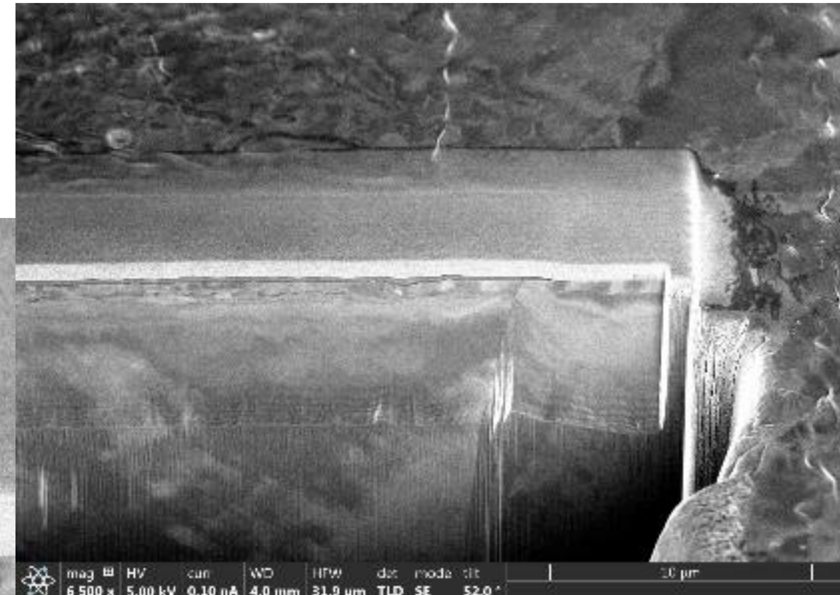


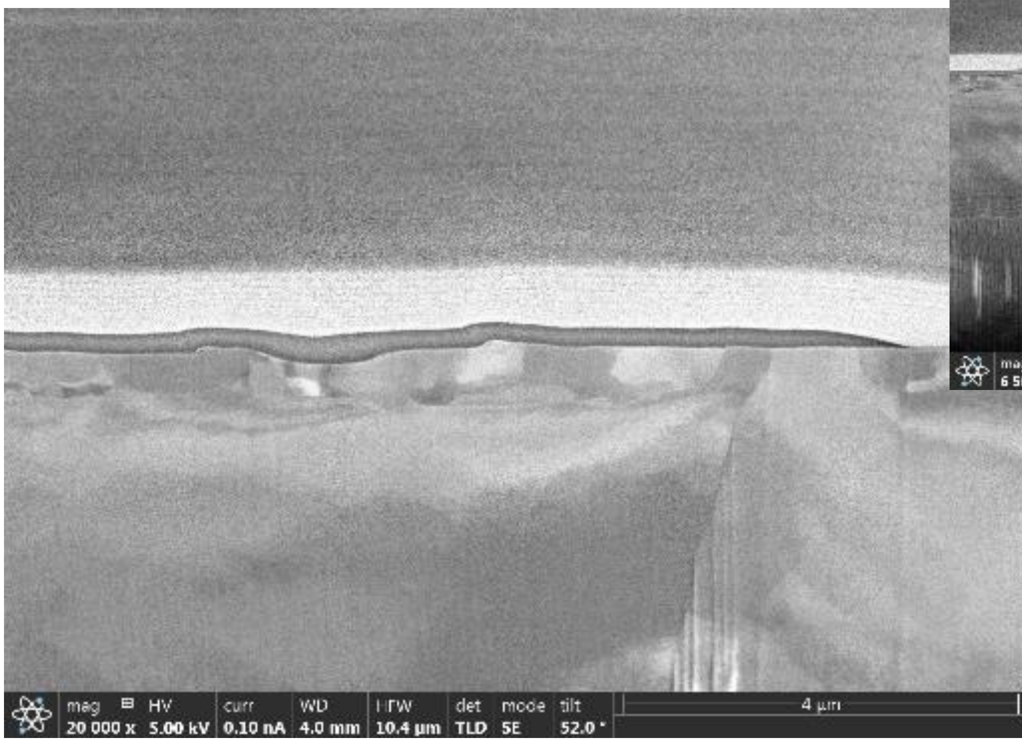
Parametrization

- 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 :
    $N\left(\frac{1}{m}\right) = \frac{\left(\frac{N_{iris}}{m}\right)\cdot(S_{iris})}{dR_{active\ regions}{}^{2}} \approx \frac{100\cdot 2\pi\cdot 2.35(mm)\cdot 1(mm)}{(10^{-2}mm)^2} = 10^7$
  - 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 : $n = \log_{1.1}\left(\frac{\tau(E)}{\tau(1.1\cdot E)}\right) \approx 30$

Cell size derived from microscopy

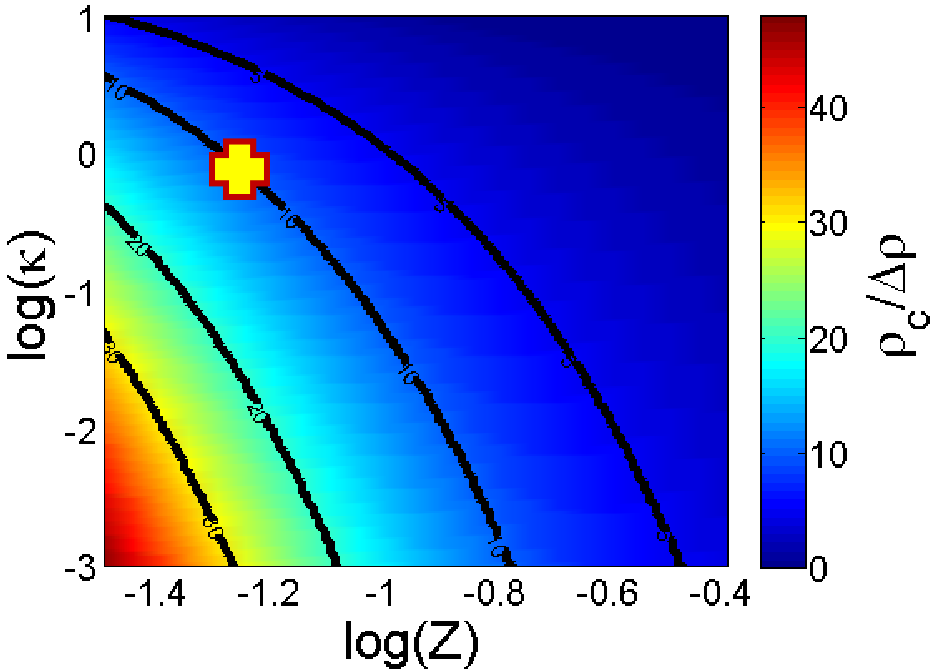


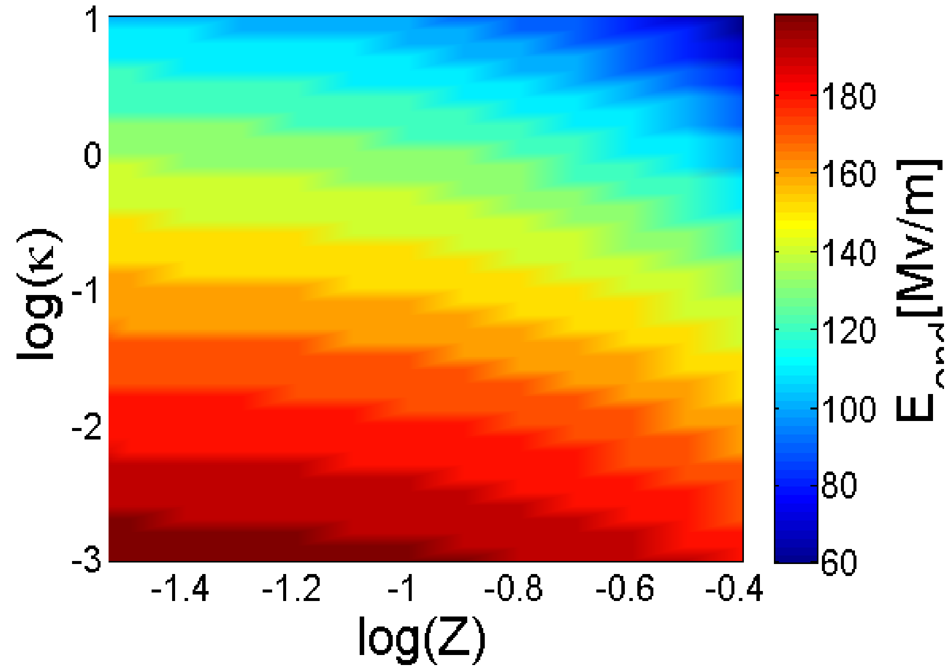


Still no clear differentiation between diamond machining effect and recrystallization
Clear top layer modifications including region with twins, slip bands localized reliefs…

Parameter space – kmc simulations

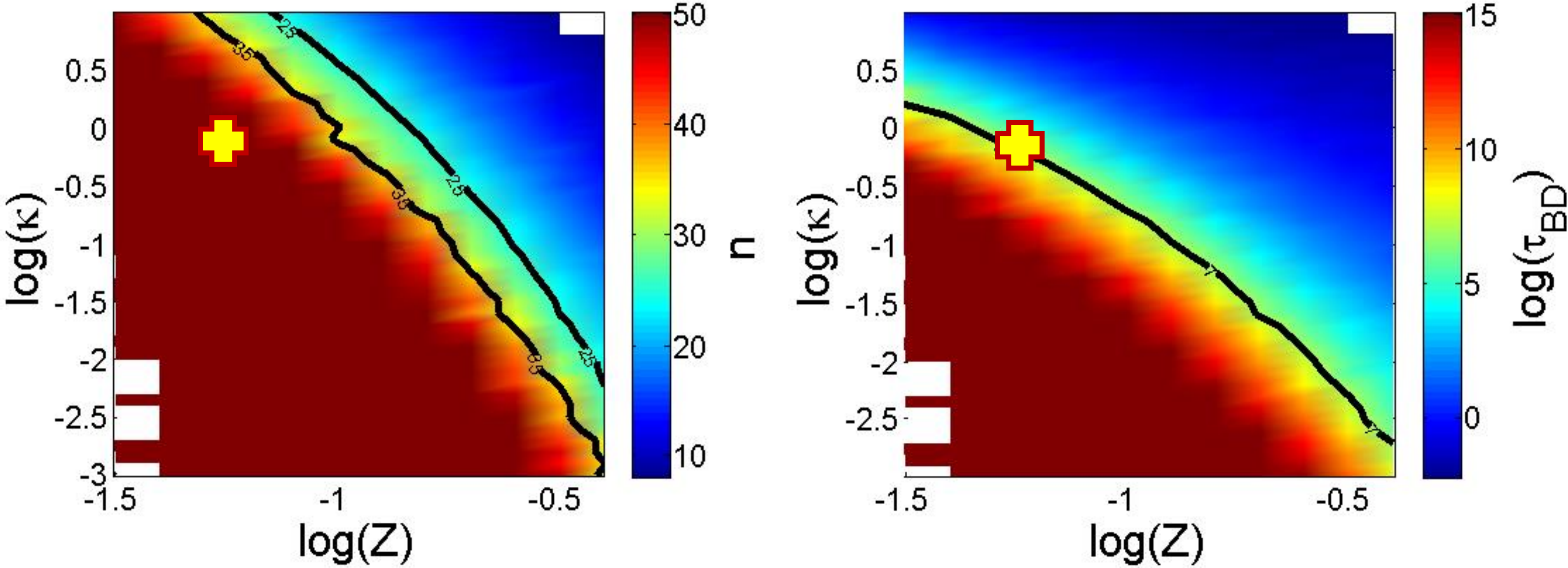
- full model validity range - using kmc





Parameter space – kmc simulations

- full model validity range - using kmc

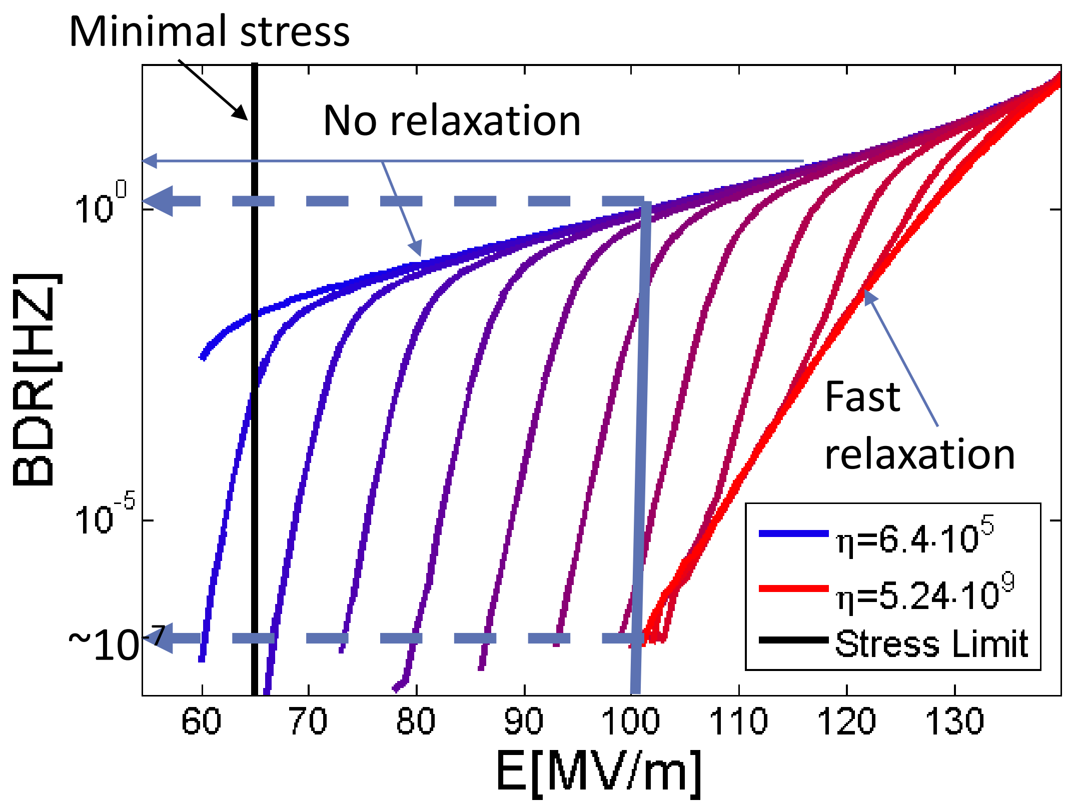


- Observable values:

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

- Significant coincidence region:

Effect of kinetic relaxation parameter

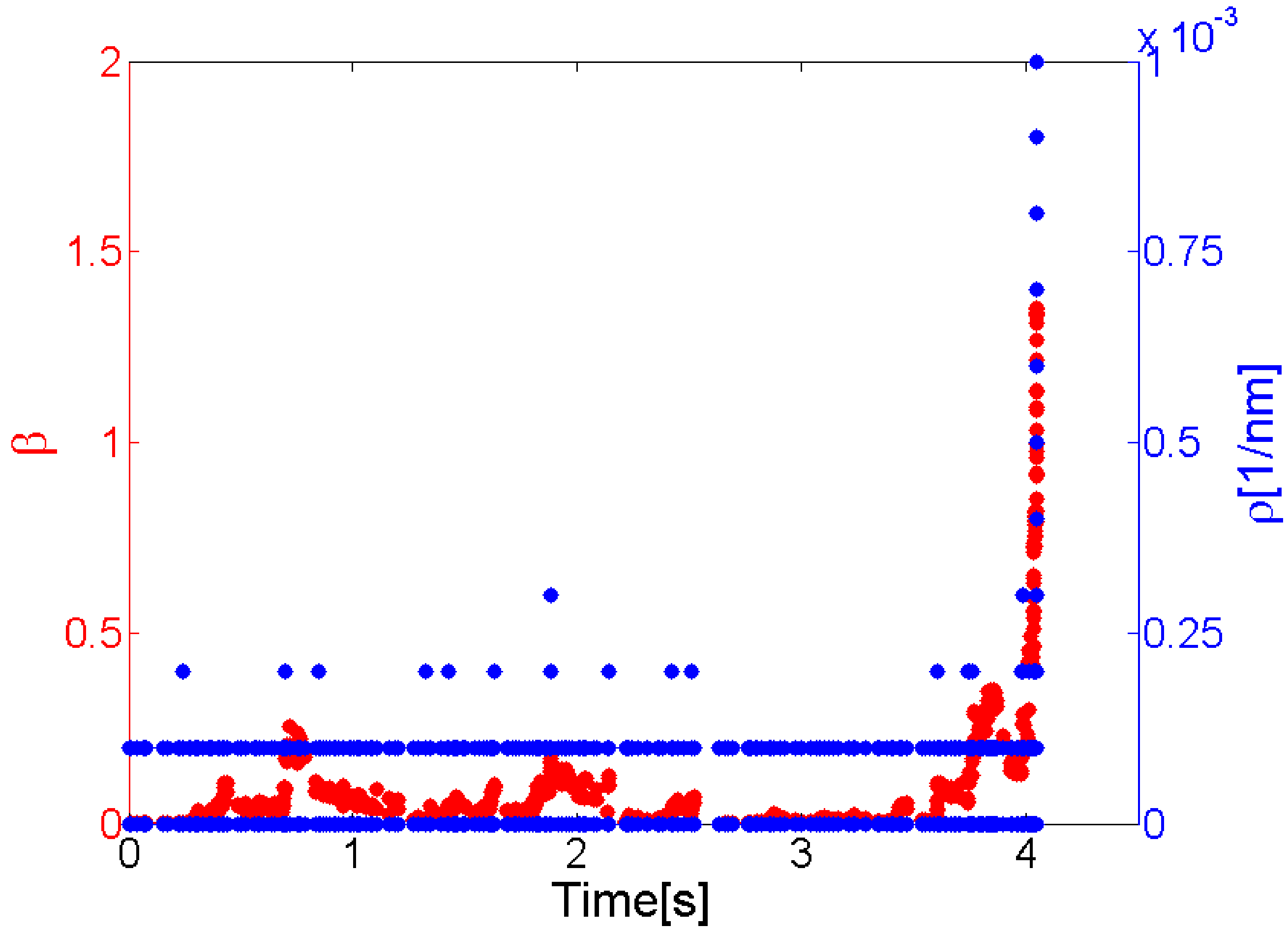


Relaxation kinetics (surface diffusion) defines two limits:

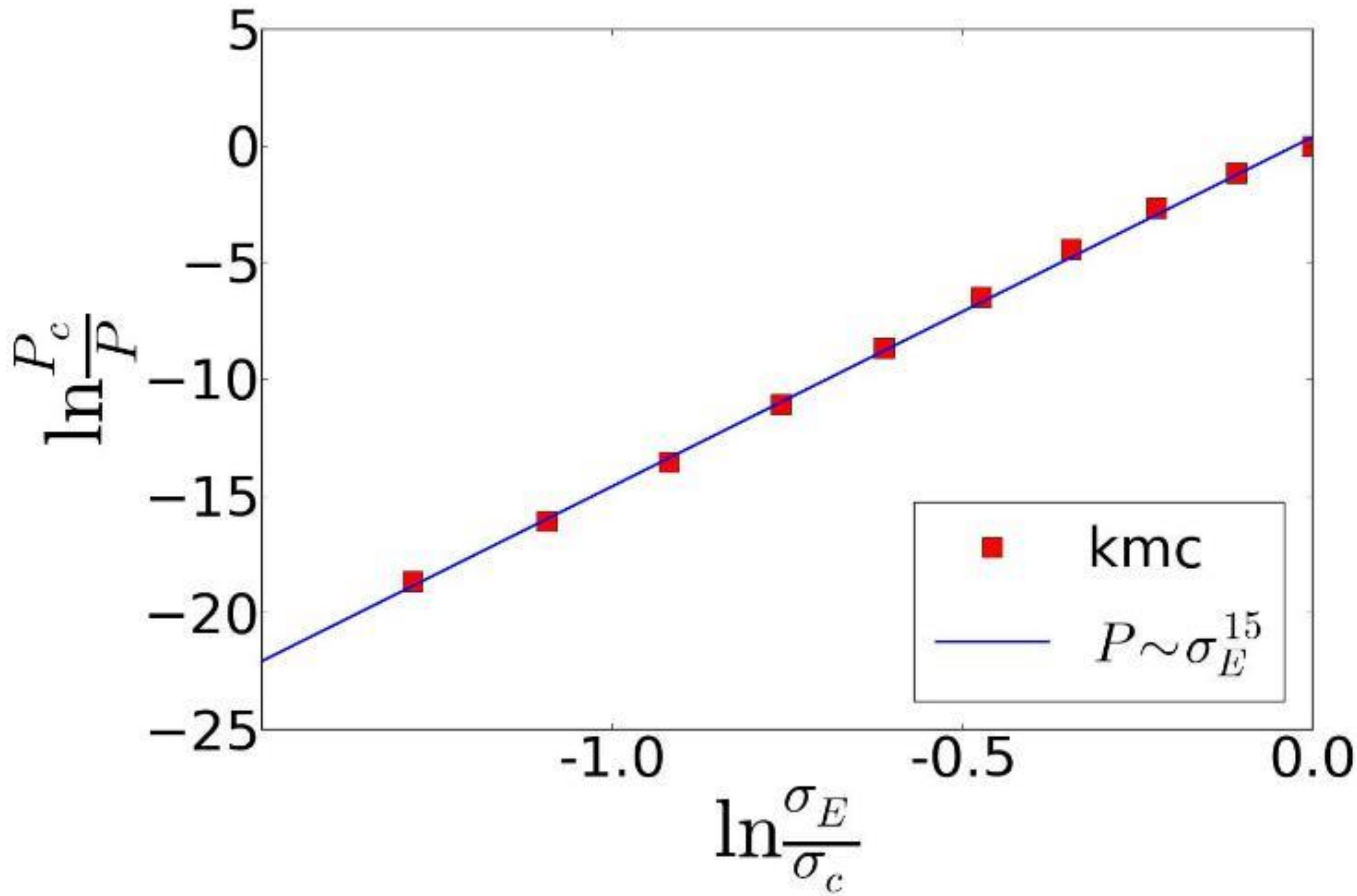
a. Fast- surface topography follows mobile dislocations content.
b. Slow- surface builds up even at metastable state of mobile dislocations .

Evolution trajectories

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



We get a power law…. (E^30)….



Signs of criticality

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

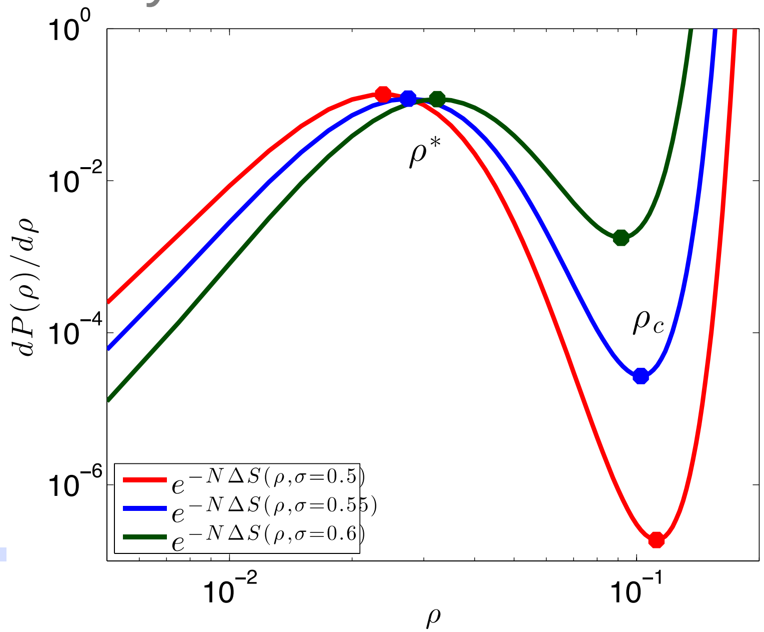
  -> identify threshold

- 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

$$SD(t) = \frac{\int_{t-\Delta}^{t+\Delta} \left(I(t) - \langle I \rangle\right)^2 dt}{\left(\langle I \rangle\right)^2}$$

- Or, more generally, autocorrelation in the signal

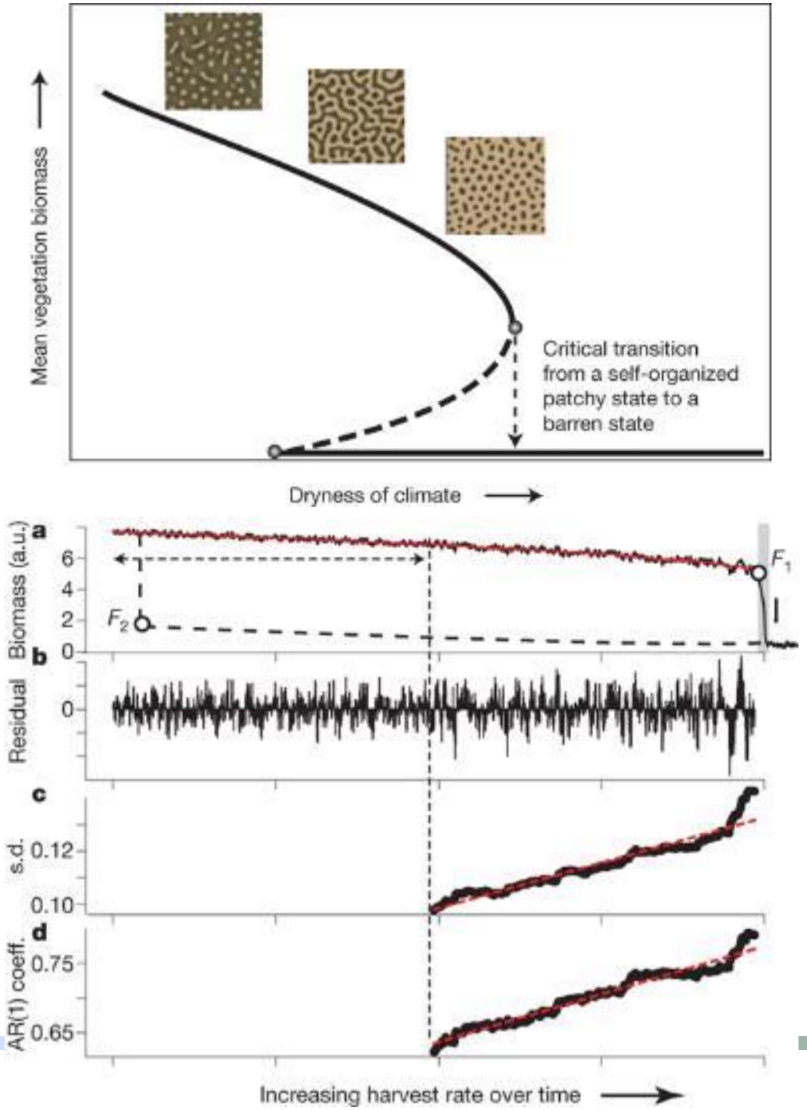
$$R(k) = \frac{\int_0^{t-k} \left(I(t) - \langle I \rangle\right)\left(I(t+k) - \langle I \rangle\right) dt}{\int_0^{t-k} \left(I(t) - \langle I \rangle\right)^2 dt}$$

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

REVIEWS

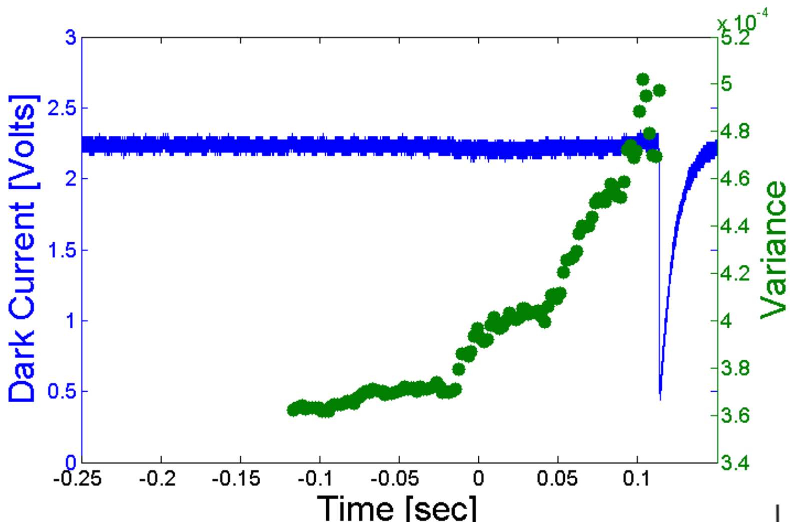
Early-warning signals for critical transitions

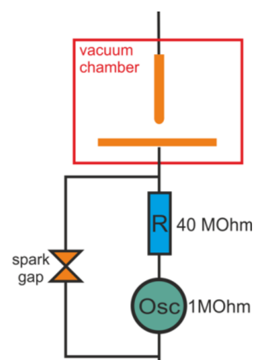
Marten Scheffer[1], Jordi Bascompte[2], William A. Brock[3], Victor Brovkin[5], Stephen R. Carpenter[4], Vasilis Dakos[1], Hermann Held[6], Egbert H. van Nes[1], Max Rietkerk[7] & George Sugihara[8]



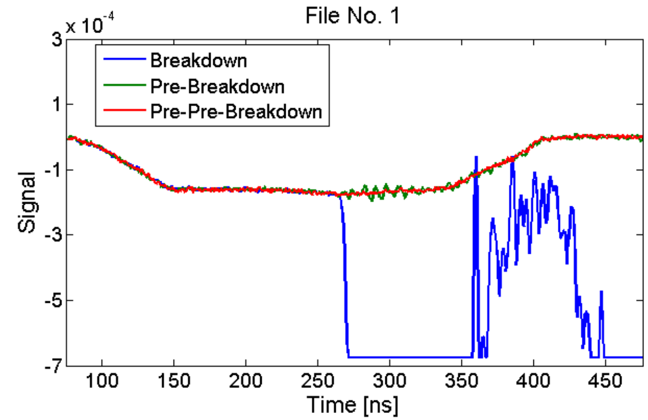
Reminder - Observations until now...

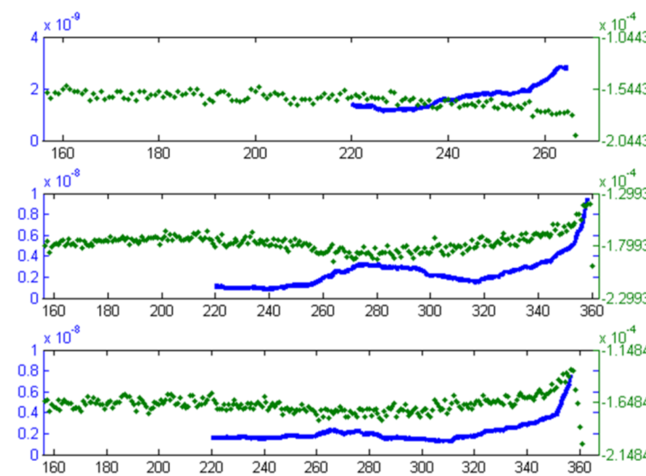
- DC and RF indications of pre-breakdown increase in dark current variance





DC data –
Iaroslava Profatilova
Tomoko Muranaka

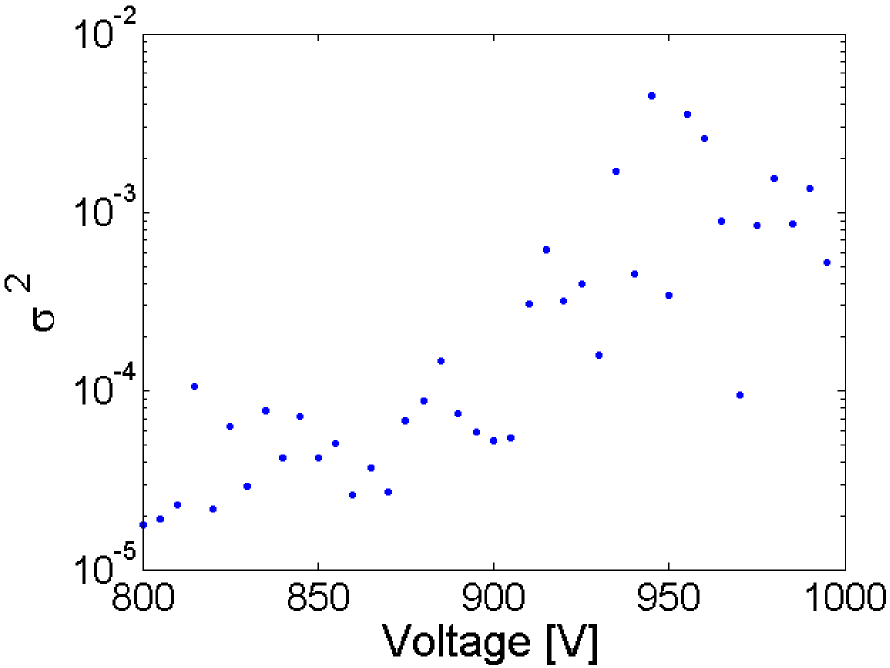


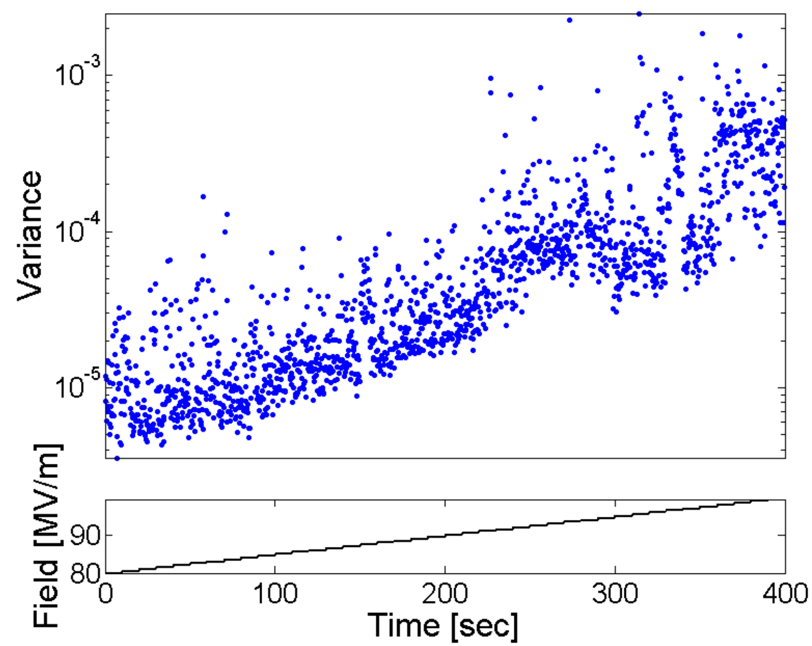


RF data - Alberto Degiovanni

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.





To compare .. We need to describe run away evolution!

Current Effort

- Improve parameterization.
- Acoustic signal prediction
- Combine functional input on:
    - kinetics of smoothing
    - Thermal stresses
- Quantify conditioning effect
- Precipitates / impurities effect

Questions:

- Kill mechanism for sub-BD events.
- Limiting parameter space
- Supporting experimental info? Can fluctuation be identified?
- Post runaway evolution…
- Will you attend mevarc 2017?!

Mevarc 2017

Save the dates: 20-23 March

Jerusalem, Israel