HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

CMS

HIP

Atomistic approach in simulations of electrical breakdowns on metal surfaces

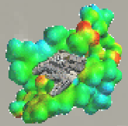
Flyura Djurabekova, Helga Timkó, Aarne Pohjonen, Stefan Parviainen, Avaz Ruzibaev and Kai Nordlund

Helsinki Institute of Physics and Department of Physics

University of Helsinki

Finland

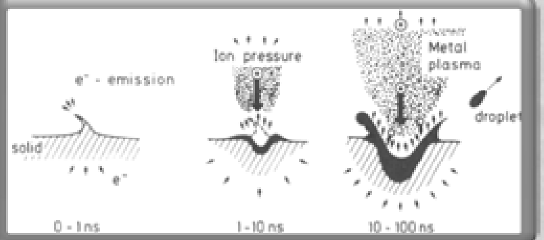
Outline

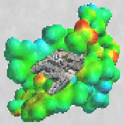


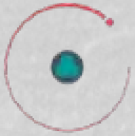
- Multiscale model to approach the problem of electrical breakdown
- Surface charge, workfunctions
- Dislocations responsible for surface response to electric fields
- Dislocation based fit model
- Summary

Multiscale model to simulate electrical breakdown

R. Behrisch, Plenum, 1986



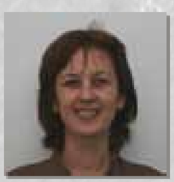




Stage 1: Charge distribution @ surface

Method: DFT with external electric field

~few fs



Stage 2: Atomic motion & evaporation
+
Joule heating (electron dynamics)

Method: Hybrid ED&MD model (includes Laplace and heat equation solutions)

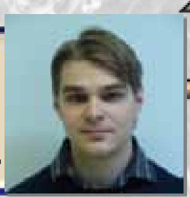
~few ns

~ sec/min

~ sec/hours

Stage 3a: Onset of tip growth; Dislocation mechanism

Method: MD, Molecular Statics.



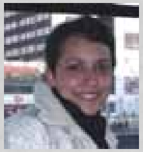
Stage 3b: Evolution of surface morphology due to the given charge distribution

Method: Kinetic Monte Carlo

Stage 4: Plasma evolution, burning of arc

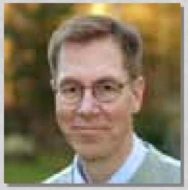
Method: Particle-in-Cell (PIC)

~10s ns

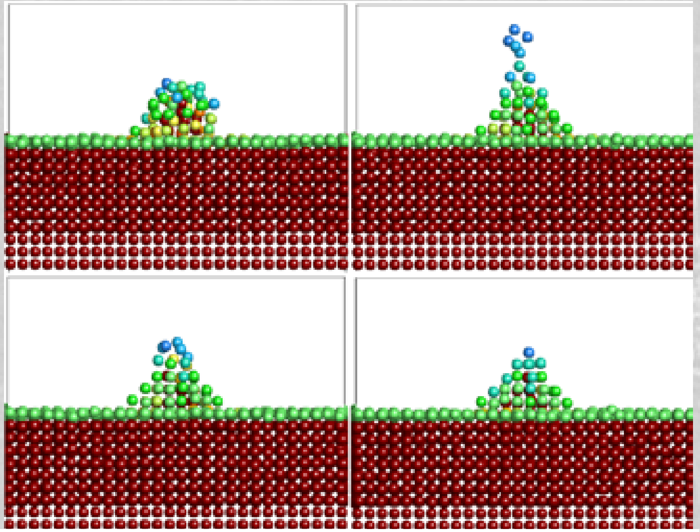


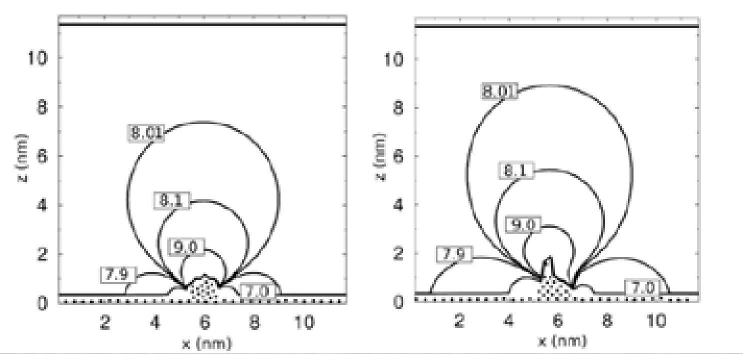
Stage 5: Surface damage due to the intense ion bombardment from plasma
Method: Arc MD

~



Evolution of a tip placed on Cu surface



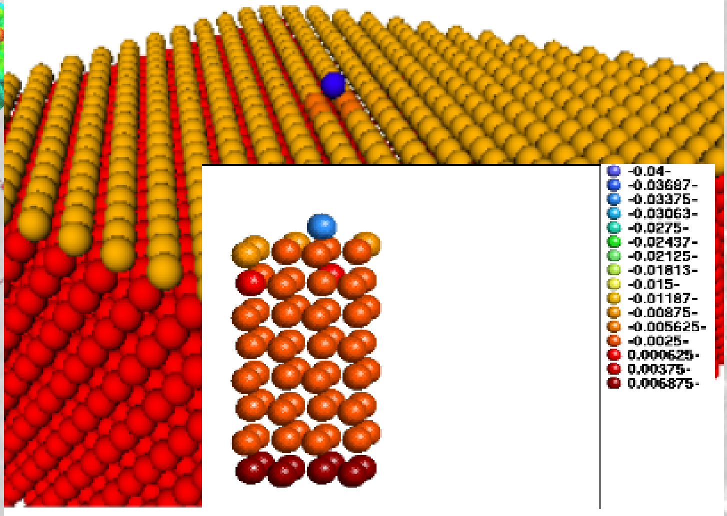


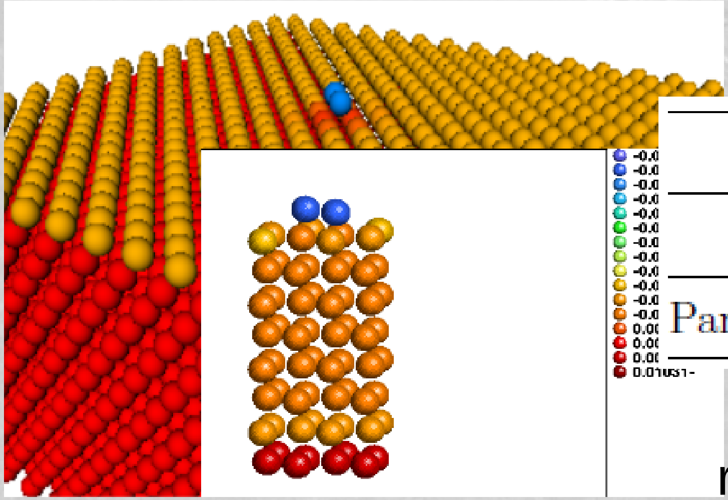
F. Djurabekova, S. Parviainen, A. Pohjonen and K. Nordlund, PRE 83, 026704 (2011).

- Follow evolution of the surfaces by calculating the partial charge induced on metal surface atoms
- The dynamics of atom charges follows the shape of electric field distortion on tips on the surface
- Temperature on the surface tips is sufficient => atom evaporation enhanced by the field can supply neutrals to build up the plasma densities above surface.

DFT calculations to validate the charges on surface atoms

$E_o = -1$ GV/m



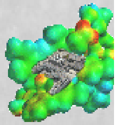


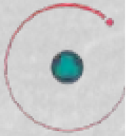
- DFT details:
  - Code: SIESTA
  - For exchange and correlations functionals the Perdew, Burke and Ernzerhof scheme of Generalized gradient approximation (GGA)
  - Slab organized in 8 layers+ 8 layers of vacuum
  - External field is added to calculate the electrostatic potential in the vacuum

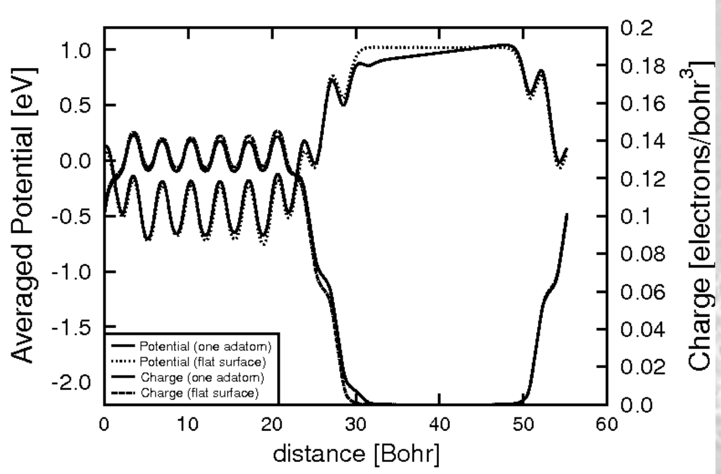
	Single adatom		Two adatoms	
	DFT	ED-MD	DFT	ED-MD
Partial Charge, q_e	-0.032	-0.0215	-0.025	-0.0177

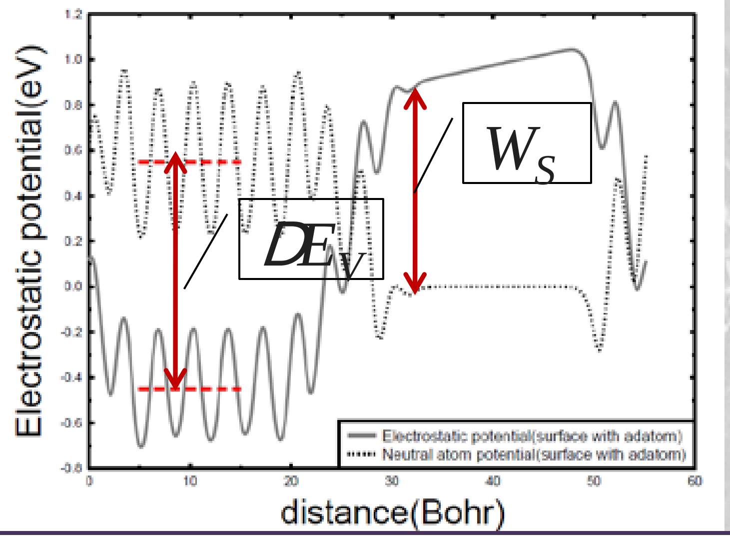
$$\sigma = \varepsilon_0 \vec{E} = 5.53 \times 10^{16} \frac{\bar{e}}{m^2} \Leftrightarrow \sigma = \frac{Q_{surf}}{A_{surf}} = 5.49 \times 10^{16} \frac{\bar{e}}{m^2}$$

Workfunction near an adatom in Cu





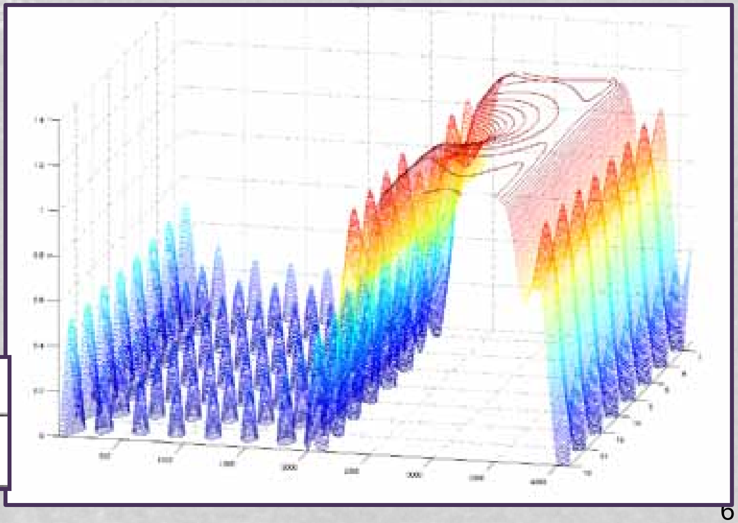




- We have calculated the workfunction for Cu surface when a single adatom is present

$$\Phi = -E_F + W_s + \Delta E_V$$

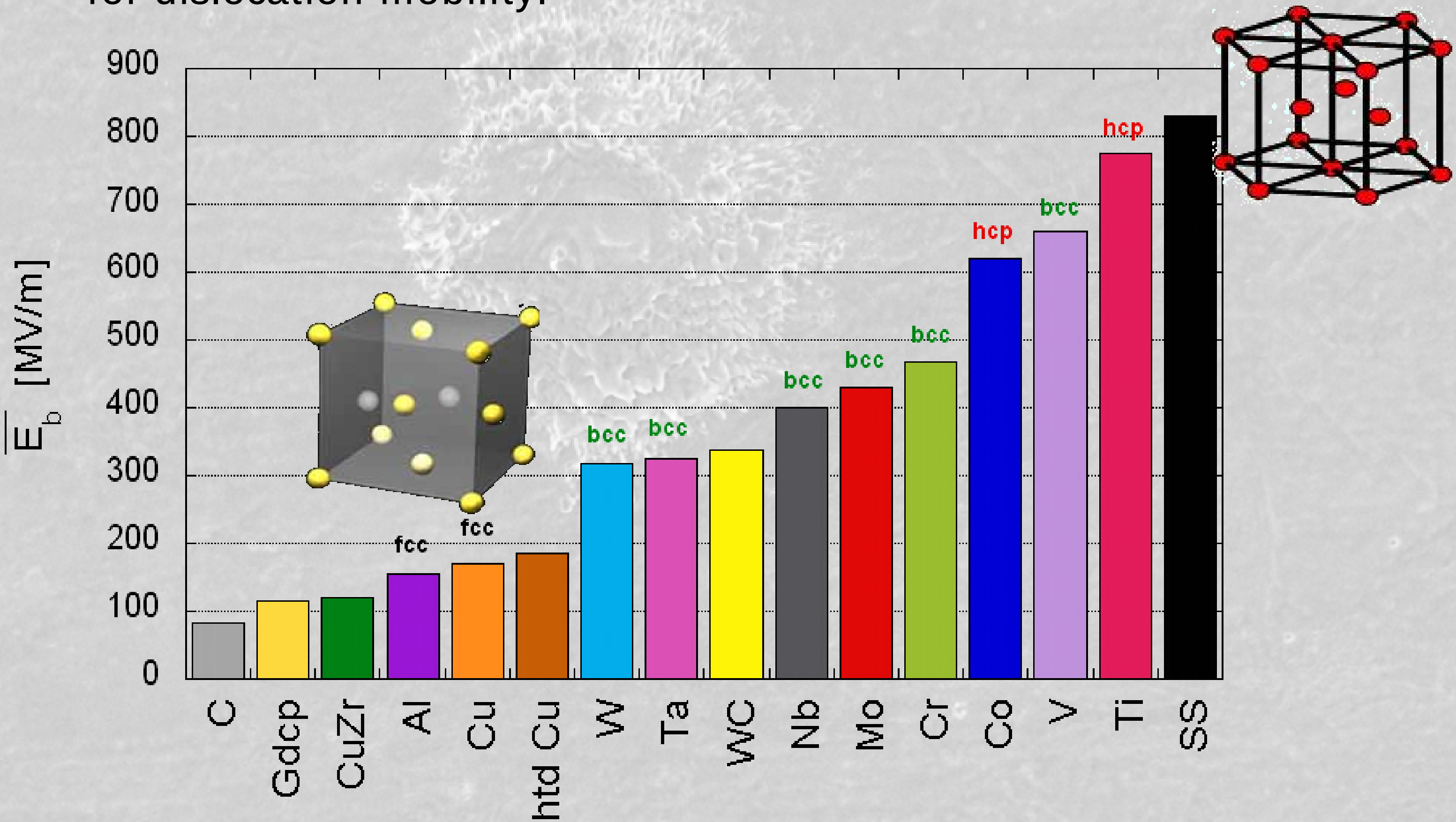
	Cu(100)	Cu(110)	Cu(111)
Φ LDA [27]	4.898	4.708	5.170
Φ(exp) [15]	4.599	4.490	4.980
Φ GGA (our calc.)	4.612	4.291	5.185



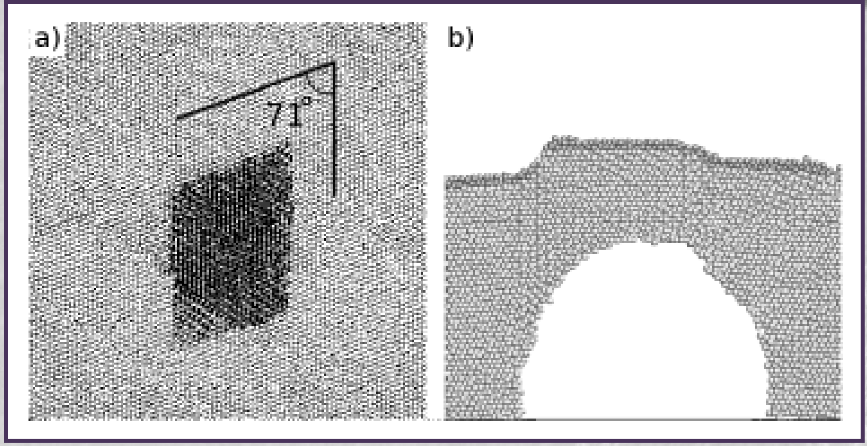
	Cu(100)	Cu(110)	Cu(111)
ΔΦ(adatom on small surface)	0.427	0.121	0.414

Motivations: why we look for dislocations?

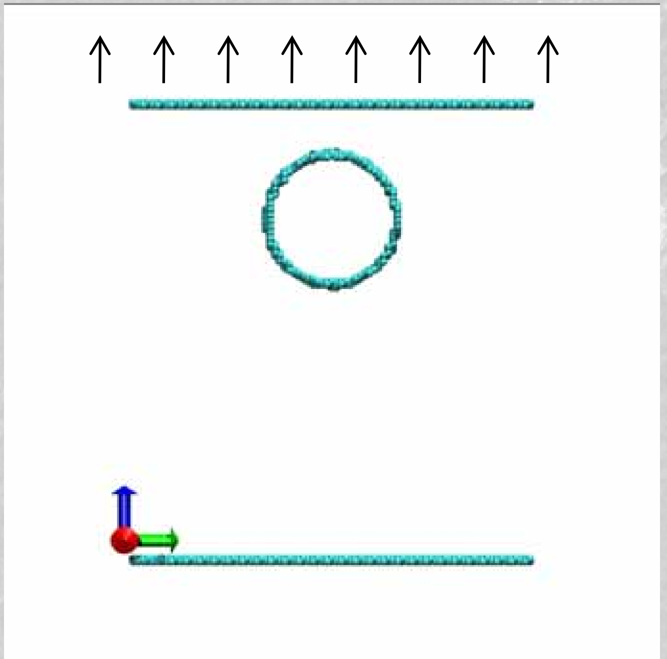
- The dislocation motion is strongly bound to the atomic structure of metals. In FCC (face-centered cubic) the dislocation are the most mobile and HCP (hexagonal close-packed) are the hardest for dislocation mobility.

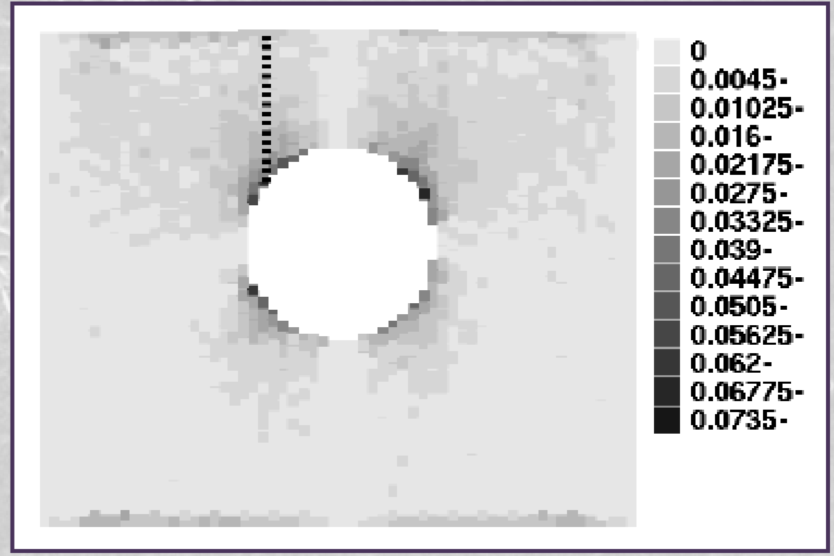


Voids: the easy way to simulate a lattice violation



- We simulated a void near {110} Cu surface , when the high tensile stress is applied on the surface. Bottom is fixed, lateral boundary allowed to move in z direction.

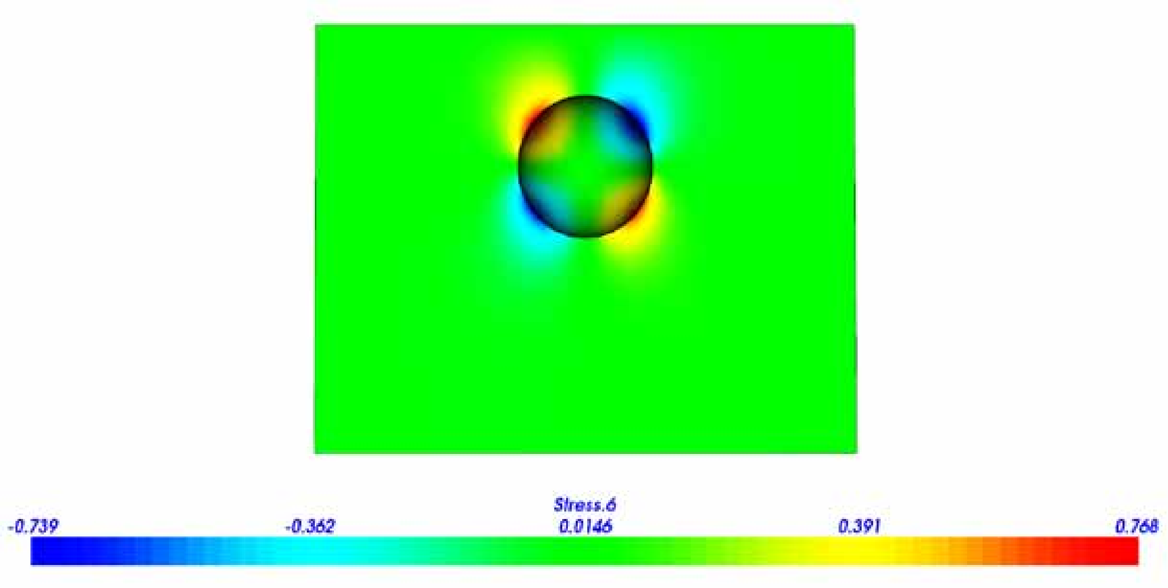


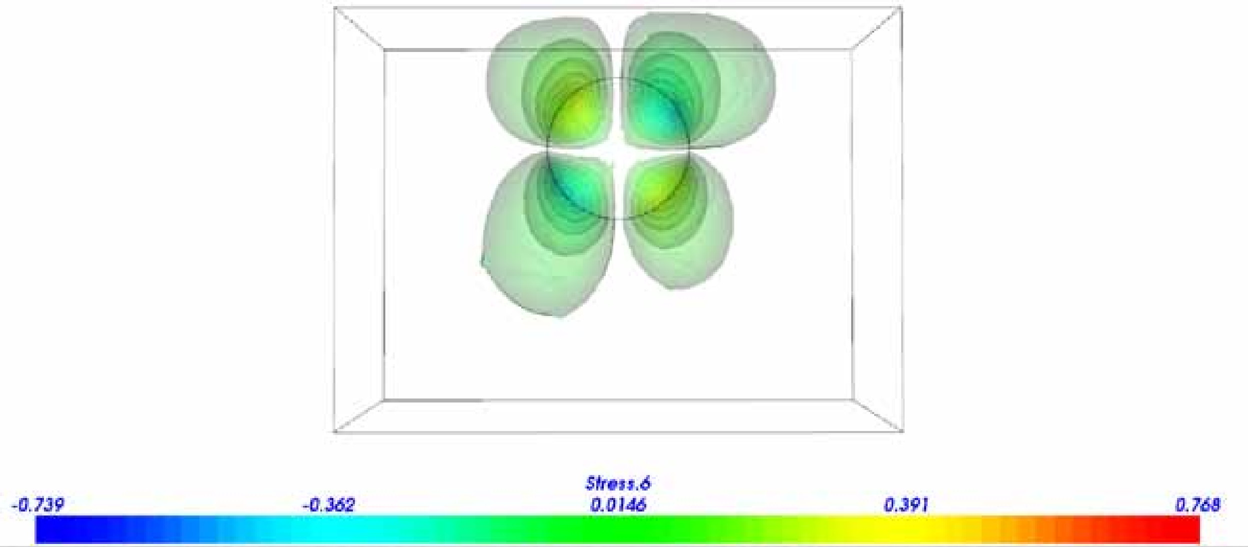


A. Pohjonen, F. Djurabekova, et al., Dislocation nucleation from near surface void under static tensile stress on surface in Cu, *Jour. Appl. Phys.* 110, 023509 (2011).

Finite Element Method calculations (ELMER)

- We have calculated the distribution of shear stresses near the void
- The shear was applied perpendicular to the surface along plane XY

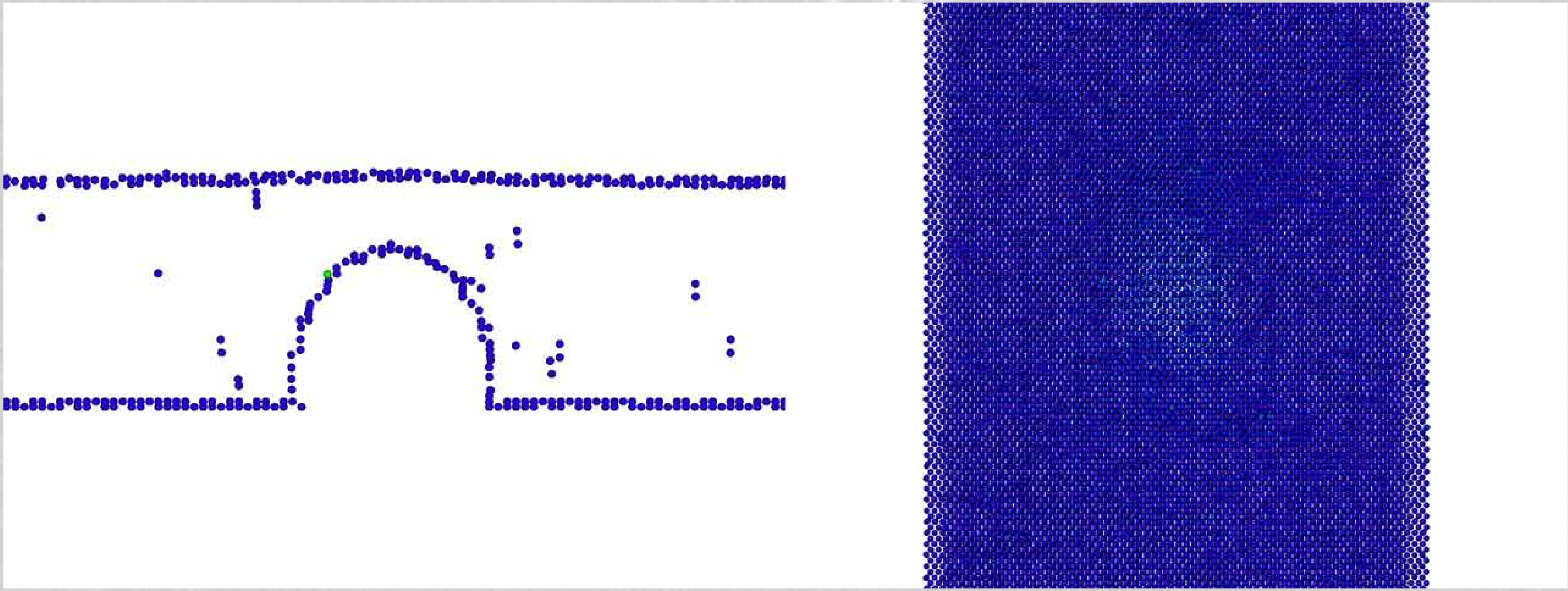




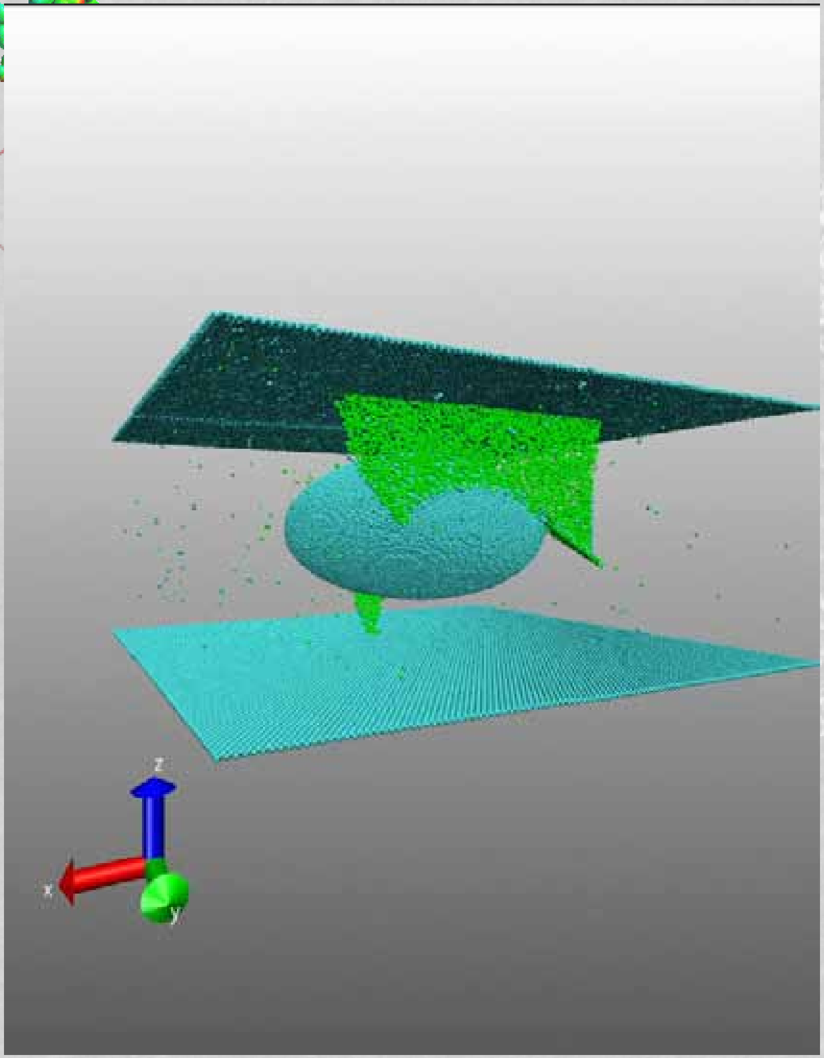
- We found a strong correlation between the maximum depth from where the void can still emit the dislocations within the MD timespan.

Concurrent ED–MD simulations of dislocations on a near–surface void

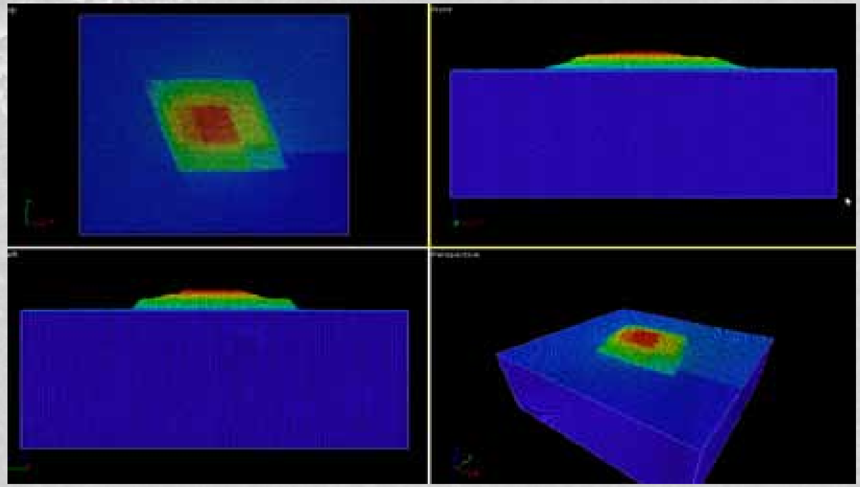
- Half-void of diameter 4nm in {110} Cu surface. (N of atoms» 170000 atoms...)
- E0=22 GV/m (exaggeration is required to simulate the dislocation within the MD time span)
- T = 600 K



If the void has the company of a screw dislocation



- A screw dislocation placed so that it intersects the void on a side, showed a cross-slip behavior leading to the atom step on the surface. This mechanism eventually combines with the previous mechanism, but to ignite this process less stress is required (in our simulations 1.7 GPa against 3 GPa).



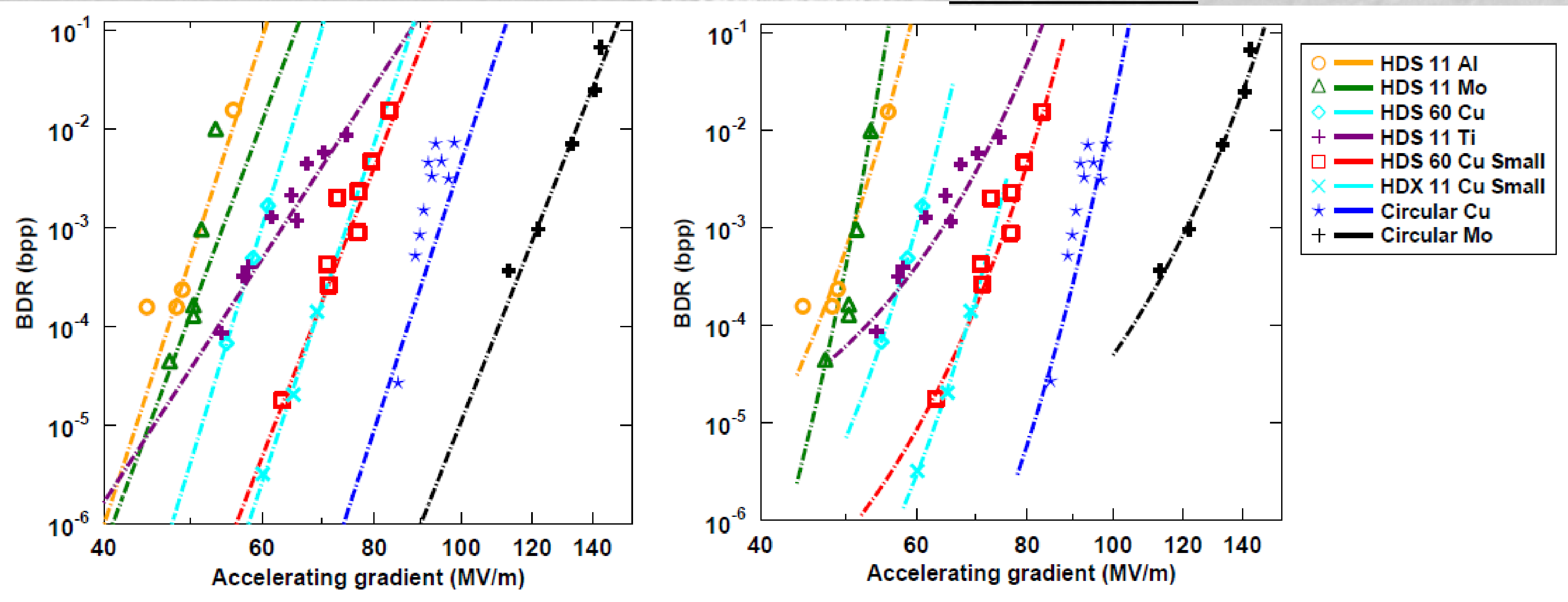
Dislocation-based model for electric field dependence

$$BDR \propto c = c_0 e^{-(E^f - e_0 E^2 \Delta V)/kT} = \boxed{c_0 e^{-E^f/kT}} e^{e_0 E^2 \Delta V/kT}$$

$$BDR = A e^{e_0 E^2 \Delta V/kT}$$

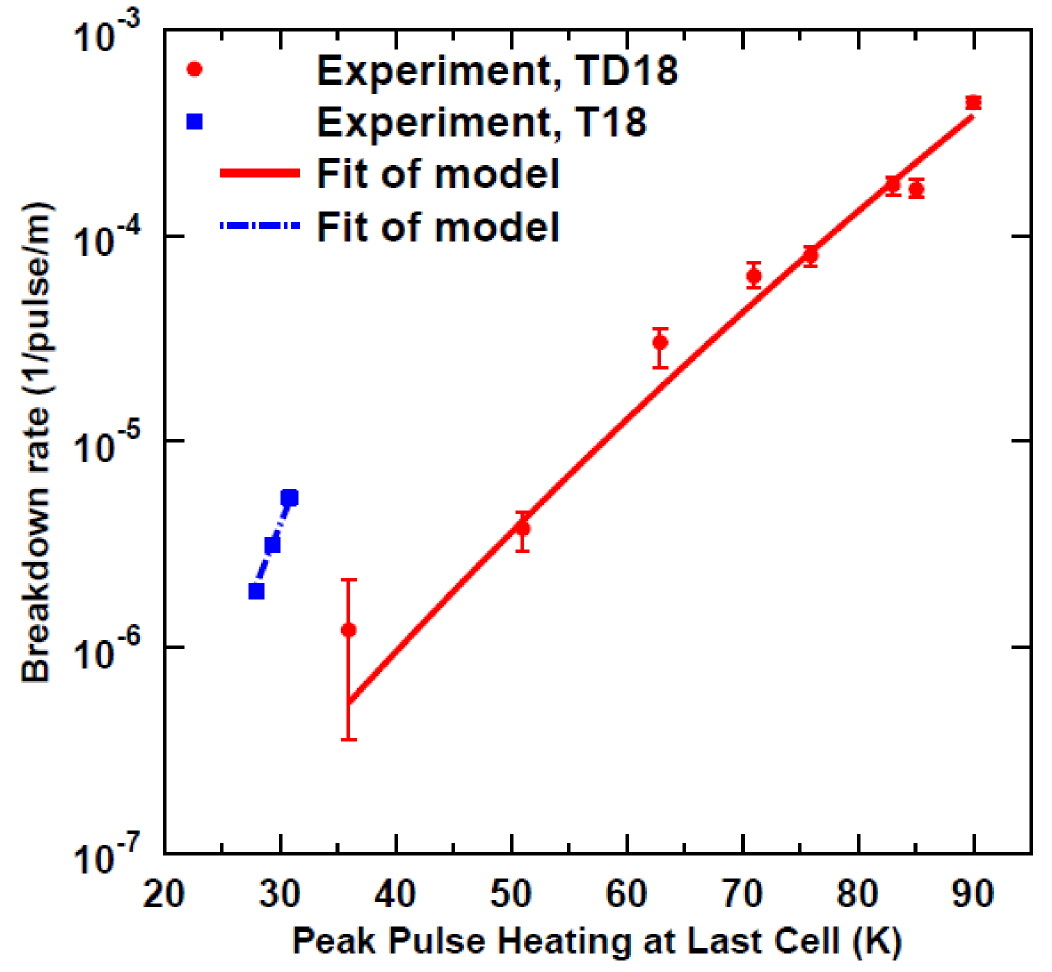
- Now to test the relevance of this, we fit the experimental data
- The result is:

Power law fit **Stress model fit**



[W. Wuensch, public presentation at the CTF3, available online at http://indico.cern.ch/conferenceDisplay.py?confId=8831.] with the model.]

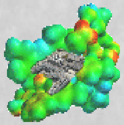
Temperature dependence of BPP



- Experimental data on dependence of breakdown rate on the peak temperature increase in accelerating components

$$R_{BD} = a' E_0 \exp\left(\frac{-E^f + \varepsilon_0 E^2 \Delta V}{k_B (T_0 + \Delta T)}\right)$$

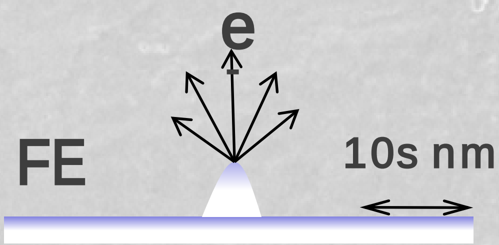
From tips to plasma:
From FE to discharge currents

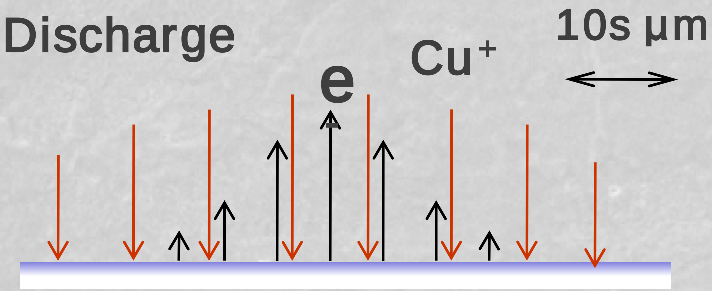


Up to 12 orders of magnitude difference

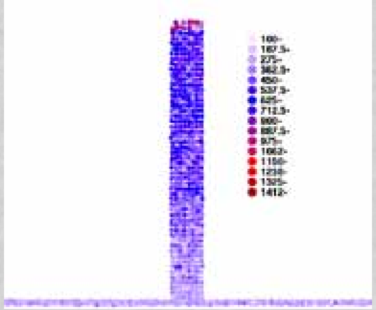
Up to 12 orders of magnitude difference

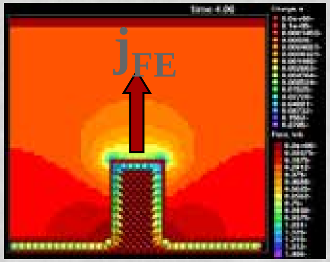
- In real life we can observe the full dynamic range of a vacuum discharge:
  - > 10s pA in ‘weak’ FE phase
  - Space charge limited ‘strong’ FE phase, typically ~ nA – μA
  - Discharge current, up to 10 – 100 A
- At the same time, the involved area changes:
  - Typically 10^{-20} – 10^{-14} m^2 for weak FE Þ R_{em} ~ 0.1 – 100 nm
  - During the discharge, the bombarded area has R ~ 10 – 100 μm



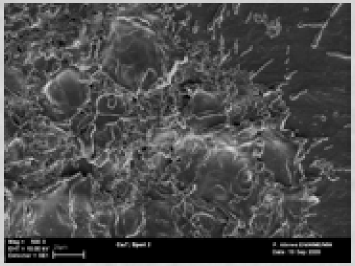


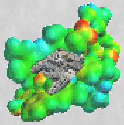
Slide courtesy of Helga Timko



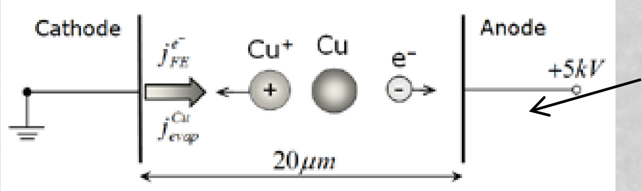


Plasma simulation



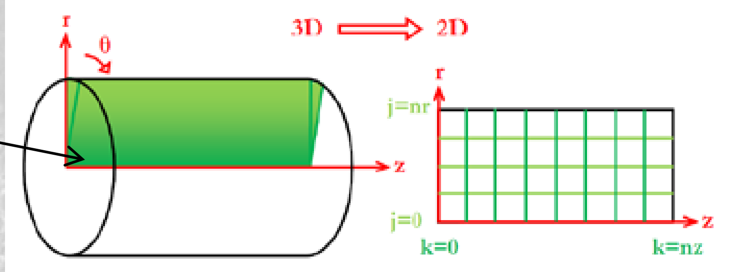


Up to now we have electrostatic PIC-MCC codes:



1D3v-model

2D3v-model



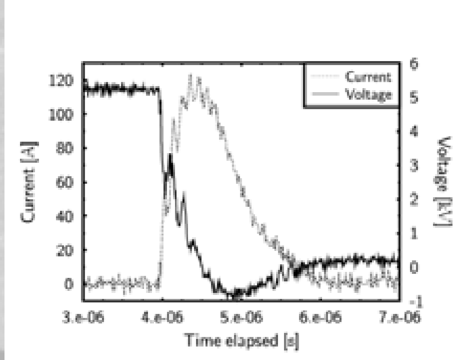
They provide us with a link between

1. Micro- & macroscopic surface processes:

   Triggering (nano-scale) ® plasma ® crater formation

2. Theory & experiments: Using reasonable physical assumptions (theory), to predict the evolution of measurable quantities (experiment)

H. Timko, K. Matyash, R. Schneider, F. Djurabekova, K. Nordlund, A. Hansen, A. Descoeudres, J. Kovermann, A. Grudiev, W. Wuensch, S. Calatroni, and M. Taborelli , ***Contrib. Plasma Phys. 5***1, 5-21 (2011)



Summary

- We develop a multiscale model, which comprises the different physical processes (nature and time wise) probable right before, during and after an electrical breakdown event:
  - All the parts of the general model are pursued in parallel. We develop intense activities to cover all possible aspects.
- Our modeling shows:
  - Plasma is fed from the tips grown under the high electric field
  - Tip growth can be explained by the relaxation of stresses inside of a material by the dislocation motion
  - A dislocation-mediated mechanism can explain the high slopes of breakdown rates against the accelerating fields


RRENT PROJECTS
N COLLISON
ONO COLLISION
A GLUONE DECECTION COLLISION
CERN
ADVANCED PARTICAL COLLIDER

Thank you!