H. Timkó[1,3] , F. Djurabekova[1], K. Nordlund[1],
S. Parviainen[1], A. Pohjonen[1], A. Ruzibaev[1], J. Samela[1],
K. Matyash[2], R. Schneider[2],
S. Calatroni[3], M. Taborelli[3], W. Wuensch[3]

[1] Helsinki Institute of Physics (HIP),
P.O.Box 64 FIN-00014 University of Helsinki, Finland

[2] Max-Planck-Institut für Plasmaphysik Teilinstitut Greifswald (IPP),
Wendelsteinstr. 1, 17491 Greifswald, Germany

[3] European Organization for Nuclear Research (CERN),
CH-1211 Geneva 23, Switzerland

E-mail: helga.timko@helsinki.fi,
helga.timko@cern.ch

Particle-In-Cell & Molecular Dynamics
MODELLING OF VACUUM ARCS

VACUUM ARCS

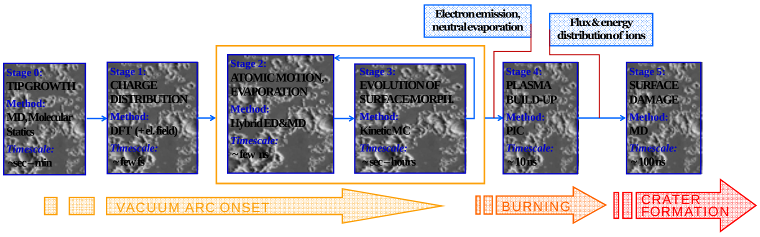
Vacuum discharges occur in a wide range of modern technology, either utilised in a controlled way, as in electrical discharge machining, or as an undesirable phenomenon from fusion reactors over satellite systems to future linear collider components. Within the CLIC project we now co-ordinate experiments and theory to explain vacuum arcs.

Vacuum arcs decrease the efficiency of CLIC accelerating structures (left).

The DC spark setup at CERN (right) serves to explore the properties of vacuum arcs in well-defined conditions.

MULTISCALE MODEL

Our group at the Helsinki Institute of Physics is using a multiscale approach to model vacuum arcs. We simulate separately the triggering of the breakdown ("onset" phase), the evolution of the plasma ("burning" phase), and the resulting surface damage ("crater formation" phase), providing a feedback between the different phases.



Electron emission, neutral evaporation

Flux & energy distribution of ions

Stage 0: TIP GROWTH
Method: MD, Molecular Statics
Timescale: ~sec – min

Stage 1: CHARGE DISTRIBUTION
Method: DFT (+ el. field)
Timescale: ~ few fs

Stage 2: ATOMIC MOTION, EVAPORATION
Method: Hybrid ED&MD
Timescale: ~ few ns

Stage 3: EVOLUTION OF SURFACE MORPH.
Method: Kinetic MC
Timescale: ~sec – hours

Stage 4: PLASMA BUILD-UP
Method: PIC
Timescale: ~ 10 ns

Stage 5: SURFACE DAMAGE
Method: MD
Timescale: ~ 100 ns

VACUUM ARC ONSET

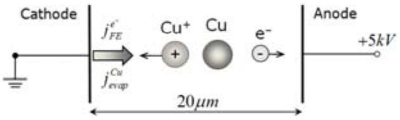
BURNING

CRATER FORMATION

The three phases of a vacuum arc: Onset, burning and crater formation.

A PLASMA FORMS

We used a 1d3v electrostatic Particle-in-Cell (PIC) code with Monte Carlo collision scheme (MCC) to simulate the early stage of plasma build-up in a DC discharge between two infinite electrodes. Three species have been taken into account: e^-, Cu, and Cu^+. Simulations assume the same conditions (voltage, gap, pulse energy) as there are in DC spark experiments at CERN.

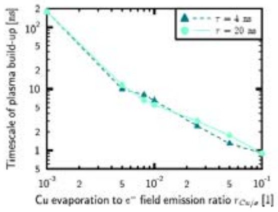


PIC simulated system. Starting from electron field emission and neutral evaporation, and taking into account impact ionisation, a plasma builds up in-between the electrodes.

As an initial condition, a field emitter with a given field enhancement factor is assumed to be present at the anode. The electron field emission (FE) current follows the Fowler-Nordheim equation.

$$j_{FE}(E) = a_{FN}\frac{(e\cdot\beta\cdot E)^2}{\phi\cdot t(y)^2}\exp\left(-b_{FN}\frac{\phi^{3/2}\cdot v(y)}{e\cdot\beta\cdot E}\right), \quad \text{where } y \propto \frac{\beta\cdot E}{\phi^2}$$

A field assisted thermal evaporation of neutrals from the field emitter following the FE current in a constant ratio $r_{Cu/e}$ is assumed too.



How the Cu evaporation to e^- FE ratio influences the timescale of plasma build-up.

THE MODEL

The following phenomena have been accounted for in this 1D model:

(i) relevant collisions occurring between the 3 species,

(ii) sputtering yields (experimentally measured, MD simulated enhanced yields, SEY etc.)

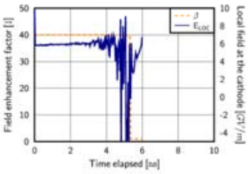
(iii) the erosion and melting of the field emitter,

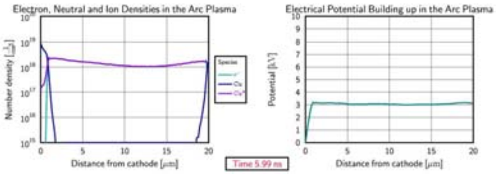
(iv) the properties of the external circuit.

BUILD-UP CRITERIA

Two criteria for breakdown can be formulated with the aid of our model: **(i)** a high enough *initial local field* – acting at a field emitter tip – to ensure growing FE current despite of space charge effects and **(ii)** reaching a *critical neutral density* – determined by the ionisation cross section and system length – to induce an ionisation avalanche.

A self-maintaining plasma: Through the sheath (bottom), a high local field (right) can be maintained even without a field emitter.



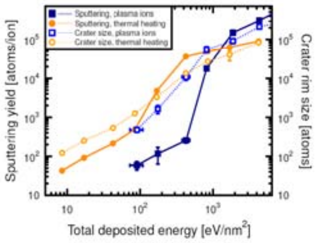


[H. Timko et al., *A One-Dimensional Particle-in-Cell Model of Plasma Build-up in Vacuum Arcs*, **Contrib. Plasma Phys.** (accepted 2010)]

SURFACE DAMAGE

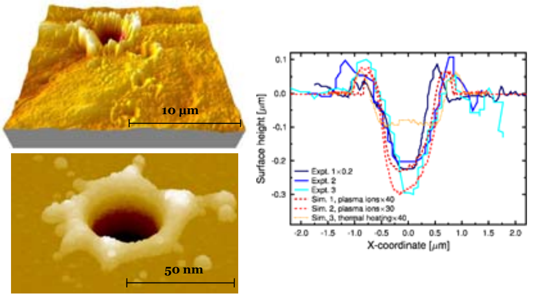
Molecular Dynamics (MD) simulations have been carried out to determine the surface damage caused by arcs. A perfect (100) Cu surface has been bombarded with Cu^+. The flux and the energy distribution of incident ions have been previously calculated with PIC, under conditions typical for the DC spark setup.

Simulations using different doses of incident ions showed that above a given threshold, the whole volume into which energy is deposited, gets melted and an enhanced sputtering starts, dominated by cluster emission.

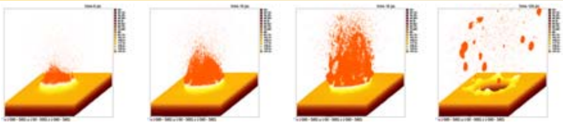


Sputtering yield and crater rim size as a function of deposited energy. The same energy has been deposited in two different ways: arc plasma (blue) and thermal deposition (orange).

[H. Timko et al., *Mechanism of surface modification in the plasma-surface interaction in electrical arcs*, **Phys. Rev. B 81, 184109 (2010)**]



Comparison of experiment (upper left) and simulation (lower left). Although simulations are limited to smaller scales, the crater depth to width ratio (right) stays constant over several orders of magnitude, in experiments as well as in simulations.



HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
MATEMAATTIS-LUONNONTIETEELLINEN TIEDEKUNTA
MATEMATISK-NATURVETENSKAPLIGA FAKULTETEN