Computer simulation of surface modification with ion beams

Zeke Insepov*, Ahmed Hassanein*, and David Swenson #

** Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL*

 # Epion Corp., Billerica MA

A U.S. Department of Energy Office of Science Laboratory Operated by The University of Chicago

Pioneering Science and Technology

Cluster Field Evaporation Mechanism of RF vacuum breakdown

Abstract

A new mechanism of RF-breakdown has been predicted by atomistic simulations of a nanoscale copper tip in a strong local RF-field consisting of tearing away a large group of tip atoms in a strong electric field that are typical for high-voltage linacs. According to these results, the energetics of evaporation makes it easier to evaporate a large group of atoms, rather than by a mechanism which goes forward consecutively, or "one-by-one", as it was previously thought. Such a group (cluster) of Cu tip material contains from 10 to 100 Cu-ions and will be evaporated within a half-period of the RF-field. Therefore, the vacuum space inside the RF-cavity would be filled by such chunks torn off from the cavity surface which is initially rough on a nanometer scale. During the next half-period of RF-field, it could strike back upon the surface, with energy of about 1KeV, thus leading to the vacuum breakdown. The obtained results are compared with the experimental data on the Field-Emission Microscopy tip fracture observations. Further experimental verification of the predicted cluster evaporation effect is discussed. .

New Mechanism of RF-breakdown in Linacs

$$F_{ev} = \frac{1}{nr_0}\left(\Lambda + \sum_i^n I_i - n\phi - \frac{3.6n^2}{r_0}\right) \text{V}/\text{A}$$

Λ, eV	ϕ, eV	r_0, Å	I_1, eV	I_2, eV	I_3, eV	E_{aff}, eV	F^{1+}, GV/m
3.50	4.60	1.25	7.73	20.29	36.83	1.23	30

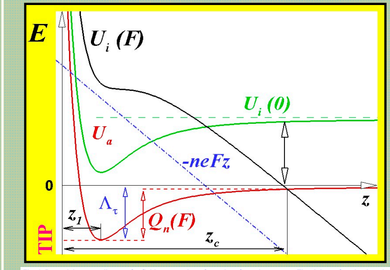
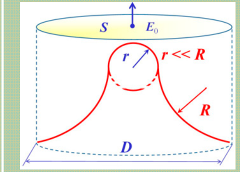


Fig. 1. Potential energy diagram for field evaporation of metal surfaces in vacuum. The tip's surface is placed on the left part of the diagram. The dot-dash line schematically shows the neutral atom potential energy U_a, the dash curve is the ion potential energy is zero field, double dot-dash straight line is the ion potential energy of the applied electric field $U_i(0)$, $-neFz$ is the energy of the charge $+ne$ in the electric field F directed toward vacuum, and the solid curve is the potential energy of an ion in the field F [2].

Metal Tip Field Evaporation Model



E_0 = 10 GV/m
$\varepsilon_0 = 8.85\times10^{-12}$ F/m
D = 55 - 125 Å
$S = \pi D^2/4 = (0.2\text{-}1.2)\times10^{-16}$ m²
$e = 1.6\times10^{-19}$ C

Gauss's Law gives:

$$N_q = Q/e = \varepsilon E_0 S/e$$

$$Nq \approx 13\text{--}66$$

Fig. 2. Schematic of the tip on the top of rf-cavity. The curvature radius at the top r is much smaller than that of the body, i.e. $r << R$. $E_0 = E'+E''$, where E' is the electric field produced by the tip and E'' is the field generated by the rest of the cavity surface. Assuming $E' = E'' = E_0/2$, we obtain the field E'' that acts on the tip's surface element. D ~ 100Å.

Temperature dependence of the RF-breakdown critical field

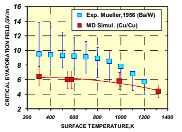


Fig. 3. Temperature dependence of critical evaporation field for removing cluster of ≈ 200 Cu ions obtained from simulation.

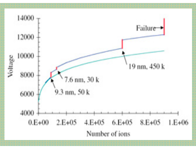


Fig 4. Abrupt discontinuities in the voltage vs. number of ions in a field evaporation system show evidence for large clusters produced at field ion microscope tips.

Field evaporated clusters are subjects to dark-current ionization

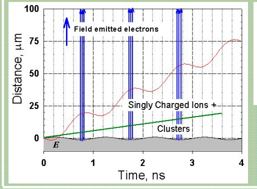
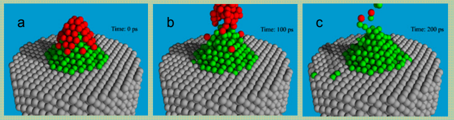


Fig. 6. Behavior of ions emitted from asperities in an electric field of 50 MV/m. The initial ion velocity comes from the local field of 10 GV/m operating over dimensions of 0.1 mm. Field emitted electrons beams are produced when the electric field reverses, and these electron beams can further ionize the ions near the emitter.

Atomistic modeling of the cluster field evaporation mechanism



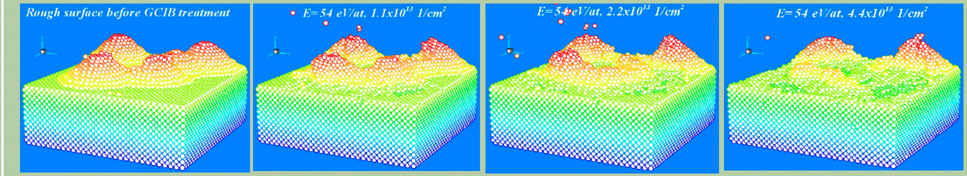
Nq charges were placed on the top of the tip, the total number of charges was constant. However, the values of each of them were changed periodically: Nq = Nm sin (ωt), ω – the field frequency. This means that the charges were following the rf-field instantaneously.

Fig. 5. Time evolution is shown of the shape of a nano-scale Cu tip on the top of rf-cavity, under a periodic electric field with maximum of 10 GV/m and frequency of 1.25 GHz at 650 K. The time instants are as follows: a) initial instant; b) 100 ps; and c) 200 ps after the start of the computation

Summary

- The RF-vacuum breakdown occurs in either copper ("warm") or niobium superconducting ("cold") cavities.
- One of the most possible mechanisms at electric field gradients as high as 10 GV/m is due to electrode surface irregularities including scratches, whiskers, crater rims, cracks, grain boundaries, oxidized areas, organic absorbed species, and dust particles.
- The cavity surface periodically have negative or positive electric potentials. During the negative half-period of the electric field, the breakdown occurs when the local field-emitted current (dark-current) density from a given site reaches 10^{11} A/m2 and causes enough heat dissipation to melt and vaporize surface material.
- Field emitted electrons could easily ionize such atomic clouds at the near-surface region and form plasma that may erode the cavity surface.
- Niobium surface modification dynamics treated by cluster ion irradiation was studied based on a Kuramoto-Sivashinsky surface dynamics equation that was further modified by adding a random crater formation mechanism. Based on the analysis of the available experimental data and existing theoretical models, a new concept of plasma formation and surface breakdown model was developed.
- Atomistic simulation model of the vacuum RF- breakdown has been developed and applied to study a picosecond-scale dynamics of the nanometer scale tip on the top of the cavity surface under applied high-voltage gradient.
- Our work showed that a new physical effect exists that consists of tearing out a small chunk (cluster of atoms) of the surface material in a high surface electric gradient and such metal clusters would fill out the near-the-surface region of the cavity.
- They could easily be ionized by the dark-current and hence hit back the cavity surface thus leading to the vacuum breakdown.
- Based on this study, a surface smoothening method is proposed consisting of the treatment of cavity surfaces by accelerated gas (argon) cluster ion beams that is capable to reducing the surface roughness up to a theoretical limit.

Atomistic simulation of Gas Cluster Ion Beam treatment



Evolution of a rough Cu surface built by placing 5 hills, with the average heights of 3.6 nm, on the top of a Cu (100) surface during irradiation with 54 eV/atom cluster ions with the following ion doses: a) initial , b) 1.1×10^{13}, c) 2.2×10^{13}, and d) 4.4×10^{13} ions/cm².

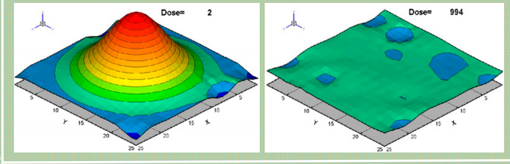
Continuum surface dynamics

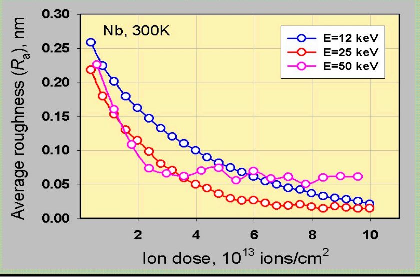
The dynamics of a non-equilibrium surface profile could be determined from the equation:

$$\frac{dh(r,t)}{dt} = \eta\nabla h(r,t) + \nu\Delta h(r,t) - k\nabla^4 h(r,t) + f_{MC}$$

η – viscosity term;
ν – surface tension term;
D_s – surface diffusion term
f_{MC} – crater formation term

$$k = \frac{D_S \gamma \Omega^2 n_0}{k_B T}$$





Dose dependence of the average Nb surface roughness for multiple Ar92 cluster ion impacts, with energies of 12, 25, and 50 eV/atom obtained by MD simulation.

AFM images of GCIB treatment of Niobium surfaces

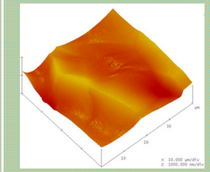


Fig. 1. Initial (unprocessed) Cornell Nb sample. (Epion MA)

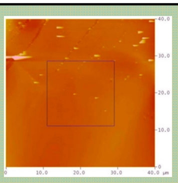


Fig.2. Processed by GCIB (NF3 + O2) (Epion MA)

Image to the left (Fig. 1) shows an initial (unprocessed) Cornell Nb sample. Altogether 9 samples were analyzed by Atomic Force Microscope before and after the cluster ion irradiation. The sample #1 (Fig. 1) had the following statistics before the irradiation: Scan size 40.00 um, Scan rate – 0.2502 Hz, Number of samples 256, Date scale 1 um. Image z-range: 288.01 nm, Image raw mean: 113.51 nm; Image Rms = 53.176 nm; Image Ra = 45.299 nm, Image Rmax = 288.01 nm. The sample #4 (Fig. 2) (after the processing by GCIB): Z-range 200 nm; raw mean 30.194 nm; Rms = 9.125 nm; mean roughness Ra = 6.289 nm; Max. height Rmax = 206.62 nm.