Ion solid interaction and surface modification at rf breakdown in high-gradient linacs

Zeke Insepov, a Jim Norem, a Seth Veitzerb

a Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439, United States
b Tech-X Corp., 5621 Arapahoe Ave., Suite A, Boulder, CO 80303, United States

Abstract. Ion solid interactions have been shown to be an important new mechanism of unipolar arc formation in high-gradient rf linear accelerators through surface self-sputtering by plasma ions, in addition to an intense surface field evaporation. We believe a non-Debye plasma is formed in close vicinity to the surface and strongly affects surface atomic migration via intense bombardment by ions, strong electric field, and high surface temperature. Scanning electron microscope studies of copper surface of an rf cavity were conducted that show craters, arc pits, and both irregular and regular ripple structures with a characteristic length of 2 microns on the surface. Strong field enhancements are characteristic of the edges, corners, and crack systems at surfaces subjected to rf breakdown.

Keywords: Ion solid interaction; unipolar arc formation; high-gradient rf linear accelerators; non-Debye plasma.

PASC codes: 29.20.-c, 52.77.Dq; 34.35.+a, 79.20.Rf; 61.80.-x; 79.20.Rf; 34.80.Dp
1. INTRODUCTION

Energetic ion collisions with solid targets are an important area of research in basic science [1-8], as well as in numerous industrial applications [9-19]. Self-sputtering processes are also of fundamental interest in the development of high-gradient rf accelerators [1]. The Neutrino Factory and Muon Collider Collaboration is looking at developing low-frequency structures for muon cooling [2–6], the International Linear Collider is optimizing the performance of 1.3 GHz superconducting rf structures aimed at the design of a 1 TeV superconducting electron/positron collider [7], and the High Gradient RF Collaboration is studying high-frequency (f >10 GHz) structures aimed at an electron-positron collider operating at energies higher than 1 TeV [8].

A self-sustained self-sputtering occurring during high-current pseudospark operation (≈ 10⁴ A/cm², I > 10⁵ A) is shown in [9,10] to be a possible mechanism for superdense glow. The self-sputtered cathode atoms become ionized in the beam of electrons accelerated in the cathode sheath.

A review of the method of MD computer simulation and results obtained for the physics of sputtering is given in [20]. MD simulations of self-sputtering and sticking coefficients of low-energy ion were reported in [21].

The goal of this paper is to develop further a new unipolar arc plasma model in high-gradient linear accelerators.

2. SELF-SPUTTERING OF SOLID AND LIQUID COPPER SURFACES

Molecular dynamics (MD) simulations of the copper self-sputtering yields were performed at various temperatures (300, 800, and 1300 K) and electric field strengths and for a wide range of Cu ion energies from 50 eV to 50 keV. The details of the calculations can be found in our previous papers [11-13] where the obtained calculated yields were compared with the existing experimental and simulation results [20-22].

Our previous OOPIC simulations¹ showed that the copper surface can become very hot as a result of ion bombardment within a few nanoseconds in close vicinity to the plasma and can be melted. Therefore, a liquid Cu surface for MD simulation was prepared by heating a copper substrate to the melting temperature of 1310 K, equilibrating this configuration, and storing it as an input file for the sputtering yield calculations. The ion energies were selected between 50 and 150 eV, corresponding to the sheath potential value obtained by our OOPIC simulation. Figure 1 shows the results of our MD simulations of self-sputtering of the copper rf-cavity surface by accelerated Cu+ ions, at ion energies varied between 50 and 150 eV and surface temperatures of 300–1310 K. The

¹ To be published elsewhere
most important result is that the self-sputtering yield at 800 K for an ion energy of 100 eV was found to be approximately 2.5 and increases as the melting point of 1310 K is reached.

The electric field affects the surface self-sputtering in two ways. One way is that the field accelerates the bombarding ion up to 100–150 eV, according to our OOPIC simulations. The second way is that a high electric field brings electric charges to the cavity surface, subjecting the surface to electrostatic tensile stress, thus making surface atoms less cohesive.

Figure 2 compares different mechanisms of surface erosion and heating that indicate an importance of the direct erosion of the surface by ion sputtering mechanism at surface temperatures above 500K.

Our simulation results show that both high temperature and high electric field can significantly increase the surface erosion. Both mechanisms will be important in a real rf cavity. We believe that the unipolar arc model explains the mechanism of surface damage in rf breakdown by increasing self-sputtering of hot copper surface residing at a very high local electric field (depending on the local curvature). This mechanism has never been addressed before in rf breakdown studies. Our simulation has showed— for the first time — that surface temperature and surface local field can significantly increase the erosion yield by a factor > 10 consistent with unipolar arcs. We note that the earliest unipolar arc model for Tokamak studies was developed based on an arbitrary assumption that the surface erosion rate was ~10 [11,12]. Here we confirm such high erosion rates at the rf cavity surfaces.

3. NON-DEBYE PLASMA FORMATION

We assume that the trigger for breakdown events is the injection of high-density material above a field emitter, where the intense, field emission currents would break up and ionize the material to produce a plasma. A number of mechanisms could be involved. Ionization of neutral metallic gas has been modeled by using OOPIC Pro, assuming field-emitted electrons are produced below an inertially confined atomic gas [23,24]. Initial results show that the ionized electrons, as well as the majority of the field-emitted electrons, are accelerated through the plasma, producing a net positively charged plasma, which is slowly expanding because of its own charge.

O00IC Pro is a particle-in-cell (PIC) physics simulation for 2D (x, y) and (r, z) geometries with 3D electrostatic and electromagnetic field solvers and Monte Carlo collision and ionization models. We model field emission at high current densities in a self-consistent way by calculating space charge fields in the presence of plasma ions and electrons. The ionization of copper and various secondary emission coefficients are contained in the code [24].
As the density of this ion cloud increases, the potential increases until it is able to trap both ionization and field-emitted electrons; but throughout the rf cycle, electrons are primarily lost to the far wall of the cavity, maintaining quasi-neutrality. As the arc evolves, simulations show that while the plasma density increases approximately exponentially, the electron and ion temperatures do not significantly increase. As the density passes $10^{24}$ charges/m$^3$, the Debye length approaches a few nanometers for electron temperatures on the order of 10 eV, and the PIC model becomes inappropriate.

For cold plasmas with densities on the order of $10^{25}$ m$^{-3}$ and electric fields less than or equal to 1 GV/m, $d_G$ is comparable to or smaller than $\lambda_D$, and the plasma is too dense to be subject to Debye screening. Under these conditions, a large area (square microns) would function like an active field emitter, subject to Fowler-Nordheim and thermal emission while being actively eroded by ion self sputtering. Modeling shows that electrons introduced into the arc would continue to ionize neutral atoms, increasing the flux of ions hitting the surface.

4. FIELD ENHANCEMENT AND SURFACE FIELDS

Defining a field enhancement, $\beta = (\text{local field}/\text{average surface field})$, considerable data shows field enhancements in the range of 100–1000 [25,26] and areas down to a few square nanometers are responsible for triggering arcs.

In addition to the structure described above, we experimentally see a variety of sharp edges, corners, and cracks in the surface. We considered field enhancements that would be present in these edges, corners, and crack systems and how they might function as field emitters. Specifically, the electrostatic Laplace equations for surface structures were numerically solved by using a finite-element multiphysics simulation package COMSOL [29]. These finite-element simulations showed that the calculated field enhancement can be comparable to the experimentally observed values $\beta \sim 140$; see Fig. 3. From the electrostatic potential of 50–100 V produced by the OOPIC simulations, which is consistent with the burn voltage of copper arcs, this results in a surface field that increases rapidly with time to values on the order of $3–6 \times 10^9$, a range of surface fields that is capable of inducing enhanced field emission, tensile failure of materials, ion bombardment, and other mechanisms of damage, even in cold surfaces (however, these surfaces would be hot because of ion bombardment).

Experimentally, high-magnification scanning electron microscope (SEM) pictures of arc pits show bubbles and ridges consistent with these high surface fields, in addition to cracks and pits with a variety of sharp edges at the limit of the resolution of the microscope. Mueller [28] and Lysenkov and Mueller [29] have also shown SEM
pictures of a variety of physical shapes that produce high enhancement factors. We assume that these sharp edges contribute to the field enhancements and thus the field emission, and we calculate their properties.

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**FIGURE 1.** Dependence of the sputtering yield of a Cu surface bombarded with Cu+ ions on ion energy, for various copper surface temperatures, $T = 300–1310$ K.
FIGURE 2. Dependence of the copper self-sputtering yields on the strength of electric field (not on ion energy – see remark at the beginning of Section 2) calculated by MD at a surface temperature of 800 K and an ion energy of 100 eV.
FIGURE 3. (a) SEM image of arc pit cracks on the breakdown surface from an rf cavity after a breakdown event showing considerable microstructure. The magnification in plot (b) shows our COMSOL simulation setting for a triple crack junction, and (c) shows the calculated field enhancement at the triple crack junction, with $\beta = 140$, consistent with cavity measurements. **ZEKE – note that the figure itself says d.**