From Field Emission to Vacuum Arc Ignition: a New Tool for Simulating Copper Vacuum Arcs

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Understanding plasma initiation in vacuum arc discharges can help to bridge the gap between nano-scale triggering phenomena and the macroscopic surface damage caused by vacuum arcs. We present a new two-dimensional particle-in-cell tool to simulate plasma initiation in direct-current (DC) copper vacuum arc discharges starting from a single, strong field emitter at the cathode. Our simulations describe in detail how a sub-micron field emission site can evolve to a macroscopic vacuum arc discharge, and provide a possible explanation for why and how cathode spots can spread on the cathode surface. Furthermore, the model provides us with a prediction for the current and voltage characteristics, as well as for properties of the plasma like densities, fluxes and electric potentials in a simple DC discharge case, which are in agreement with the known experimental values.

1 Introduction

Vacuum arc discharges can occur under several circumstances, from fusion devices [1, 2] to satellite systems [3, 4]. In particular, they are the main limiting factor for the high-gradient cavity performance of future particle accelerator designs, such as the Compact Linear Collider (CLIC) [5-7]. Given the high electric surface fields that are present in the room-temperature CLIC cavities, we restrict ourselves to discharges initiated by electron field emission [8].

The “life cycle” of vacuum arcs, which includes initial field emitter formation, cathode spot formation, the burning of the arc, and the possible formation of new spots, was described phenomenologically several decades ago [9]. Recently, much new insight has been obtained with modern computer simulation methods [10-14]. However, creating a full model of this life cycle requires the use of several simulation techniques to describe the different processes involved, which occur on different length- and time-scales. We attempt to do this with a combination of density functional theory, molecular dynamics, particle-in-cell (PIC) and hybrid simulation methods [15-17]. This paper focuses on modeling the initial plasma build-up in vacuum arcs using PIC.

Modeling this plasma build-up is a necessary and important step towards a full model. Firstly, plasma build-up serves as a link between theory and experiment, as it can estimate measurable quantities such as the voltage-current characteristic, densities, etc. Secondly, it links the triggering and the surface damaging phases. Interestingly, both the field emitter formation – a nano-scale, transient phenomenon [18], and the crater formation – a macroscopic, visible effect [19], are materials science

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processes, while the link between them is determined by plasma physics. Thus, modeling the plasma build-up in vacuum discharges is a challenging task of describing the transition from a microscopic to a macroscopic phenomenon. A close relation to materials science and surface processes is therefore indispensable.

The essence of studying the plasma initiation lies in the plasma-surface interaction occurring at the cathode spot. This cannot be simulated with existing, powerful PIC codes, as they lack the material science capabilities required for this particular problem. Our earlier 1D PIC model [11] gave a good insight into the plasma properties of the high-density core, but it cannot describe the spatial distribution of particles, nor the related plasma dynamics. Hence, we developed a new tool, the 2D ArcPIC code, for simulating vacuum arc initiation. This tool is capable of describing the formation and spreading of a cathode spot, starting from field emission.

This paper is organized as follows: after a description of the experiments to be modeled in Sec. 2, the numerical methods and the physics model of the 2D ArcPIC code are presented in Sec. 3. Simulation results are shown and discussed in Sec. 4, before the concluding remarks in Sec. 5.

2 Experiments to be modeled

In order to better understand radio-frequency (RF) discharges that occur in accelerating cavities, direct current (DC) vacuum arc discharges are studied in a well-defined, controlled manner using the CERN DC spark experiment setups, described in [18–21]. Typical discharge conditions in these setups (external electric field, vacuum pressure, energy available to the breakdown etc.) have been adjusted to match the conditions encountered in RF. The modeling is for the time being also focused on these well-defined DC vacuum arcs. In the description below, we shall mention some experimental facts and observations which are relevant to our theoretical model.

In the DC setup, vacuum arcs are generated between copper electrodes under ultra-high vacuum (UHV). A typical electrode gap distance is 20 µm. With copper electrodes, breakdowns usually occur at an applied voltage of about 4–6 kV [22], or in terms of the surface electric field, around $E_z = 200–300$ MV/m. This is also the typical maximum surface field in the CLIC accelerating cavities [7,23].

Prior to breakdown, a current consisting of field-emitted electrons is observed. This current is described by the Fowler-Nordheim equation [24–28]

$$I_{\text{tip}}(E_z) = A j_{\text{FN}}(E_{\text{loc}}) = A \kappa_1 E_{\text{loc}}^2 \exp \left( \frac{-\kappa_2}{E_{\text{loc}}} \right),$$

(1)

where $A$ is the emitting area, $E_{\text{loc}} = \beta E_z$ is the local field on the emitter, and $\beta$ is the field enhancement factor. Using the Wang and Loew approximation [28] and assuming a work function of 4.5 eV, which is an average for polycrystalline Cu [29], the factors $\kappa_1$ and $\kappa_2$ take the values $\kappa_1 = 4.7133$ A/GV$^2$ and $\kappa_2 = 62.337$ GV/m. The field enhancement factor $\beta$ and the emitting area $A$ can then be found via measurements of the field emission current at multiple field levels $E_z$, by fitting the data to the Fowler-Nordheim equation. Typical measured values for $\beta$ are in the range 30–60 [22].

An interesting observation about copper is that breakdown always occurs around a “critical” local field of $E_{\text{loc}} = 10–11$ GV/m [30]. Since the Fowler-Nordheim equation has an exponential dependency on $\beta$, the contribution of the surface protrusion with the largest $\beta$ will dominate the field emission current, and thus the local field can be interpreted as the electric field prevailing locally above the strongest field emitter site in the probed area.

From field emission to a fully developed vacuum arc, the experimentally observed range in current and area spans more than 10 orders of magnitude. Field emission currents and field enhancement factors are typically measured in the 0.1–1 nA range, while in a fully developed discharge, a current of up to 10–100 A may be present. Correspondingly, the areas that are involved in the process may be as small as $10^{-2}–10^{-2}$ nm$^2$ [18] during the field emission phase, as determined from a fit to the Fowler-Nordheim equation, whereas final damaged areas reach the size of $10^6–10^{10}$ nm$^2$ [19].

In our DC experiments, the energy available to the discharge is stored in an external transmission line that is initially charged to high voltage. The energy range that can and has been investigated using..
our setup is about 1 mJ to 1 J \cite{31}, with 15 J being the typical energy stored in a CLIC RF pulse \cite{5}. However, RF measurements indicate that the energy absorbed by a breakdown might be only a tiny fraction of the stored energy \cite{32}, as most of the incident RF pulse is reflected by the breakdown plasma.

Investigating different materials, it has been observed that the breakdown field, field enhancement factor, and local field are determined by the cathode material only: measurements using a tungsten anode in combination with a titanium cathode and vice versa gave the same results as measurements carried out with both electrodes being made of the cathode material \cite{22}. This confirms that vacuum arcs in our setup are cathode-dominated, as one would expect for room-temperature electrodes \cite{33}.

In light of the above, we aim at developing a plasma model that would describe how a microscopic phenomenon (the initial field emission) can turn into macroscopic surface damage (due to the ion bombardment). Our model takes into account that the power and energy available to the arc is limited, and at the same time includes the plasma-surface interaction at the cathode. This makes it possible to model the early-stage current-voltage characteristic of a vacuum arc, which currently cannot be precisely measured due to bandwidth limitations in the DC spark experiment. Similarly, we can also make predictions for the ion bombardment and electric fields under the footing of the arc, which are difficult to access experimentally.

### 3 Methods and code description

The 2D ArcPIC code \cite{34} is specifically developed for the purpose of modeling vacuum arc discharges. It is an electrostatic PIC code equipped with Monte-Carlo collision routines. The material properties and external circuit characteristics are described by modular classes, which allows for the study of different models. Particles are described in a five-dimensional phase space with two coordinate and three velocity components (2D3V), assuming cylindrical symmetry. A uniform grid is applied to the simulation domain’s \((r, z)\)-plane, where \(r\) is the radial and \(z\) the height coordinate of a cylindrical coordinate system. As a consequence of the cylindrical coordinate system, the volume element \(dV = 2\pi r dr dz\) increases linearly with radial distance, which is taken into account when calculating the densities and solving the Poisson equation.

The phase space for the particles is continuous, while macroscopic plasma quantities are discretized onto grid points. The self-consistent electrostatic field includes both the external electric field and the space charge contributions. The code’s finite difference method (FDM) Poisson solver uses the SUPERLU package \cite{35,36} for matrix inversion, which provides an efficient solution of the sparse matrix problem with the aid of the lower-upper factorization method. The particle mover uses the Boris method \cite{37,38}, which is an implicit solver. For the field interpolation to particle position and the charge assignment to grid points, we use the first order cloud-in-cell scheme \cite{38}. Using the same field interpolation as charge assignment scheme on a uniform grid ensures momentum conservation \cite{39}.

#### 3.1 Stability and limitations of the PIC implementation

Since we are simulating a runaway process, but the dynamic range of PIC in density and temperature is limited, the time step \(\Delta t\) and grid spacing \(\Delta z\) have to be appropriately chosen. To ensure that the dynamic range is not exceeded, the fulfillment of basic stability criteria \cite{39} for \(\Delta t\) and \(\Delta z\) are regularly verified in the code. Furthermore, the full dynamic range of vacuum arcs (1 nA–10 A) cannot be covered; this limitation is circumvented by assuming a rather strong field emission (0.005–0.01 A) initially and limiting the maximum current through the choice of parameters for the external circuit, as discussed in Sec. 3.5.

The simulation of a transient, non-linear problem, for which direct comparison with experiment is limited or unavailable, is a complex task even for a well-tested code. However, progress in code validation can be made via code-to-code comparisons. Within the framework of a code-to-code benchmarking effort with the previous 1D model \cite{40}, we have uncovered that several details of the physics model, such as charge assignment, interpolation methods for the impact ionization cross-section data, etc. can affect the time-to-breakdown. Therefore, in the present paper, we mainly aim at a qualitative description of vacuum arc ignition.
3.2 Collisions

Modeling the early-stage evolution of vacuum arcs, the code treats only the three most relevant species: electrons, Cu neutrals and Cu$^+$ ions. To treat collisions between particles, collision routines have been adapted from a 1D PIC code developed at the Max-Planck Institut für Plasmaphysik \cite{39,41,42}. Collisions are carried out according to a Monte Carlo algorithm, based on concepts developed for the direct Monte Carlo simulation of rarefied gases \cite{43,44}. The following reactions are implemented with experimentally measured, energy-dependent cross sections in the code (see \cite{45} for a detailed description):

- Coulomb collisions between the pairs (e$^-$, e$^-$), (Cu$^+$, Cu$^+$), (e$^-$, Cu$^+$) \cite{46},
- Elastic collisions e$^-$ + Cu $\rightarrow$ e$^-$ + Cu \cite{47},
- Impact ionization e$^-$ + Cu $\rightarrow$ 2 e$^-$ + Cu$^+$ \cite{48},
- Charge exchange and momentum transfer Cu$^+$ + Cu $\rightarrow$ Cu + Cu$^+$ \cite{49},
- Elastic collisions, Cu + Cu $\rightarrow$ Cu + Cu.

Impact ionization is a decisive factor for plasma build-up in vacuum arcs, as seen in Sec. 4. For its implementation, we use an algorithm that is similar to the null-collision method described in Ref. \cite{50}. However in our algorithm, for every electron in the cell, a neutral is chosen to collide with. For each of these electron-neutral pairs, the collision probability is calculated and compared to a random number $R \in (0, 1)$ in order to decide whether or not the collision takes place.

3.3 The surface model

The surface model is responsible for removing the particles leaving the domain, and injecting new particles into the domain. As illustrated in Fig. 1 the relevant processes are field emission processes and sputtering processes.

3.3.1 Field emission and neutral evaporation

A cylindrical field emitter of area $10^4 \text{ nm}^2$, corresponding to a radius $R_{\text{tip}} = 56.4 \text{ nm}$, is assumed to be located at the cathode, around the symmetry axis. The field emitter is assumed only implicitly through particle injection routines; no assumptions on a particular shape or other properties of the field emitter are made. This field emitter is assigned a field enhancement factor $\beta_{\text{tip}}$, and serves as a source of electron field emission and Cu neutral evaporation. For the simulations presented in Sec. 4, we chose $\beta_{\text{tip}} = 35$, corresponding to an initial local field $E_{\text{loc}} = \beta E_z \approx 10 \text{ GV/m}$ as in the experiments. Since in reality surface roughness and smaller emitters are practically unavoidable, we also assign an average field enhancement factor $\beta_{\text{flat}}$ to the “flat” cathode surface, which is the area outside of the central field emitter region. For both the “tip” and the “flat” region, the electron current densities are calculated

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using the Fowler-Nordheim equation (Eq. 1), where a cut-off of $E_{\text{loc}} = 12 \text{ GV/m}$ is applied for the field emission. This cutoff is based on the validity range of pure Fowler-Nordheim field emission [8] from a copper surface.

Since the field emitters are exposed to a very high $E_{\text{loc}} = \beta E_z$ and a current density $j_{\text{FN}}(E_{\text{loc}})$ that can heat up the emission region significantly, the field emitter also serves as a source of neutrals and ions through a mixture of thermal and field evaporation [51, 52]. In the present plasma simulations, we introduce the parameter $r_{\text{Cu/}}$ which is the ratio between evaporated Cu neutrals and field-emitted electrons. In our case, the neutral evaporation is a field-assisted thermal process, which is motivated by atomistic simulations. Our studies indicate that atoms from the emitters can be ripped off due to the local electric field [12, 16] and as a result of strong electron currents (electromigration). For most simulations, this ratio was set to $r_{\text{Cu/}} = 0.015$, which is just high enough to produce a breakdown within 3 ns, which is the maximum run length of the simulations presented here. This value for $r_{\text{Cu/}}$ is similar to those explored in [11].

3.3.2 Sputtering and secondary electron yield

Besides field emission and neutral evaporation from the field emitter, as well as field emission from outside the field emitter, several sputtering phenomena are taken into account:

- High-energy ion impacts can cause the emission of electrons at the cathode. Above an ion impact energy of 100 eV, we apply a constant secondary electron yield (SEY) of 0.5.
- Single Cu and Cu$^+$ impacts sputter Cu at both the anode and the cathode with an experimentally measured, energy-dependent physical sputtering yield [53].
- Based on earlier molecular dynamics studies [10], an enhanced sputtering yield is expected in the dense region of the arc footing, where ions are bombarding the cathode surface with a high flux that is above a certain threshold value [1]. A plausible mechanism that could cause such an increased sputtering is a combination of electric field [54] and thermally-enhanced [55] sputtering, since the arc induces both a high field and a high temperature at the surface. Studies are ongoing to determine the exact yield and threshold for the ion energies reported in this paper.

In the simulations presented here, we investigate the effect of different enhanced yields ($Y_{\text{enhanced}} = 0, 1, 2$) and threshold fluxes ($j_{\text{enhanced}} = 10^{24}, 10^{25}, 10^{26}$ particles/cm$^2$/s). This high-flux sputtering model is applied on top of the empirical energy-dependent single-impact sputtering, taking into account all ions and neutrals with a kinetic energy above 23 eV, which is the lower cutoff of the energy-dependent sputtering.

For further details on the SEY and a discussion on possible other surface phenomena that may play a role, see [11].

3.4 Particle injection

For the current $I_{\text{tip}}$ originating from the field emitter “tip”, we inject the particles over an area with radius $R_{\text{emit}} = 0.4 \mu\text{m} > R_{\text{tip}}$. Since no physical process can be resolved on a scale which is smaller than or similar to the grid spacing, which in our case is comparable to $R_{\text{tip}}$, the particles have to be injected over at least a few grids. In this way, we also ensure that numerical stability is maintained. On the other hand, we cannot simply increase $R_{\text{tip}}$, as this would result in unphysically high field emission currents. In the simulations, the local field and hence the field emission current density are matched to experimental values, thus the area also needs to be of a similar order of magnitude as experimentally observed. Injection is carried out with a uniform density of injected particles above the injection area. Neutrals are injected in the same manner as electrons, where the number of neutrals injected equals the

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1 We previously saw that when bombarding a copper surface with a high ion flux and impact energies around 5 keV, and also when directly assigning thermal energies to the surface atoms (matching the same total deposited energy as in the bombardment), a strongly enhanced surface sputtering was triggered [10]. Although the average impact energy in the current studies is much lower than in these simulations, we investigate the effect of enhanced sputtering due to the high fluxes and elevated temperatures on the surface under the cathode spot.
number of electrons times $n_{Cu/e}$. In addition to the injection of particles from the “tip”, we also inject field-emitted and evaporated particles from the “flat” part of the cathode ($r > R_{tip}$).

For SEY and single-impact sputtering, particles are injected from the same position as the incident particle. For high-flux sputtering, the position of the produced particles is sampled over a radial Gaussian distribution such that the $\sigma$ of this distribution is the outer edge of the outermost cell where the bombardment flux was greater than the threshold $j_{enhanced}$.

The initial velocities of the electrons and neutrals are sampled from Gaussian distributions corresponding to temperatures of 0.29 eV and 14.5 eV, respectively. The distributions are truncated, removing parts with low velocity and negative $v_z$, in order to avoid very large densities building up near the surface. The neutral temperature was chosen to match the typical temperature of sputtered atoms, which is $O(10 \text{ eV})$ [56]. This temperature is also used for neutral evaporation, where the elevated temperature causes the neutrals to leave the injection region quickly, maintaining numerical stability in the grids near the surface.

### 3.5 Circuit model and potential boundary conditions

In a real system, the initial high voltage across the gap cannot be maintained forever, but will start to drop as current is drawn from the system and energy is consumed. We assume a circuit as shown in Fig. 2 which is similar to the current DC spark circuit [20, 21]. This model contains a local gap capacitance, and an infinite remote energy supply which can only be accessed through a resistor. The gap voltage is thus given as

$$V_{\text{gap}} = V_{t=0} + \frac{1}{C_{\text{gap}}} \int_0^t (I_{\text{circ}} - I_{\text{gap}}) \, dt \ , \text{ where } I_{\text{circ}} = \frac{U - V_{\text{gap}}}{R} \text{ and } V_{t=0} = U \ . \ (2)$$

Fig. 2 The circuit model used in the simulations, which is a simplified version of the circuit in the experiment. It consists of an external load $R$, an external voltage supply $U$ and the capacitance of the discharge gap $C_{\text{gap}}$.

We chose $R = 1000 \ \Omega$ and $C_{\text{gap}} = 1.0 \ \text{pF}$ as our reference parameters. These are close enough to the equivalent parameters of the real circuit ($C_{\text{gap}} \approx 10 \ \text{pF}$ and $R = 100 \ \Omega$) so that much of its behavior can be reproduced. However, the higher resistance and lower capacitance in the model yields a lower peak current and smaller stored charge, significantly reducing the required run-time, making it possible to run the simulation until depletion of the stored charge.

The gap current $I_{\text{gap}}$ is calculated using the Shockley-Ramo theorem [57,58], which takes into account that the charged particles in the gap induce charges on the cathode and anode. This keeps the displacement current $I_{\text{cap}}$, which is due to removal of the charges induced by the externally applied field, separate from the gap current. Using this method to calculate $I_{\text{gap}}$ has the effect of smoothing the current signal seen by the circuit model, compared to using the charge crossing the cathode surface each time step.

### 4 Simulation results and discussion

In this section we present and discuss the results of our simulations. In Sec. 4.1 a detailed description of the “reference” simulation is presented, and the obtained quantities are compared to experimental data where this is available. The effects of varying some of the parameters are shown in Secs. 4.2 and 4.3 with focus on the surface parameters and the spreading of the arc in Sec. 4.2 and focus on the circuit...
parameters and the evolution of the current and voltage with time in Sec. 4.3. The parameters of the simulations are listed in Tab. 1, where the bold numbers are the reference values of a parameter in cases where this parameter is varied in Secs. 4.2 and 4.3.

4.1 Reference simulation

While the experiments have a typical gap size of \( Z \approx 20 \, \mu m \), we use a narrower gap of \( Z = 6 \, \mu m \) in the simulations. At the same time we lower the supply voltage to \( U = 1740 \, V \), keeping the initial field at \( E_z(t = 0) = 290 \, MV/m \). This matches the typical experimental conditions, while reducing the computational demands.

The voltage and current characteristics of the simulated transient are shown in Fig. 3(a), and the particle sources and sinks as a function of time in Fig. 4. The flux of ions arriving on the cathode surface as a function of time and \( r \) is presented in Fig. 5(a), while Fig. 5(b) shows the energy spectrum of the ions. The electric potential (Fig. 6), the particle densities (Fig. 7) and the velocity distributions (Fig. 8) are plotted at a set of characteristic moments in time.

To start from Fig. 3(a) in the simulation the two currents \( I_{circ} \) and \( I_{gap} \) can be distinguished, while experimentally only \( I_{circ} \) can be measured. Comparing the simulated current and voltage curves to the experimentally measured ones in Fig. 3(b), we see that the time scale and shape of the current- and voltage curves are similar between the experiment and the simulation. Much of the remaining differences can be explained by differences between the experimental and the simulated circuit, as discussed in Sec. 4.3. One can break down the evolution of the discharge into the three main phases, which are visible in Fig. 3(a):

1. For about 1.0 ns in the beginning (Figs. 6(a) and 7(a)), the field emission is relatively weak and the current more or less constant. Only a few neutrals are present in the system at this stage (since sputtering is negligible), gradually forming a cloud of high-density gas above the field emitter. Hence, until the very end of this stage, ionization is rare and localized to a small region. However, if the initial field emission is strong enough, the space charge screening can be overcome with the aid of the first ions appearing in the cloud. The local field at the emitter then grows slightly (Figs. 6(b) and 7(b)), leading to a significant rise in field emission current due to the exponential nature of the Fowler-Nordheim equation (Eq. 1).

2. When this happens, the emission of both electrons and neutrals rapidly increases, leading to a sequence of events. First, when locally a high enough neutral density is reached, the electron mean free path of the impact ionization becomes small enough to start an ionization avalanche in the plasma cloud. Since electrons move fast, the plasma quickly becomes quasi-neutral. Hence, a plasma sheath appears, which enhances the local field above the emitter.

3. The creation of the plasma sheath greatly enhances the field above the surface, triggering strong emission from the “flat” surface as well. This marks the transition from the breakdown to the volume-defined arc discharge phase. As seen in Fig. 3(a) this occurs around 1.2–1.3 ns.

Concerning the surface processes, the ionization avalanche quickly creates a large number of ions, which are accelerated across the newly created plasma sheath (Fig. 6(f)). This leads to heavy bombardment of the surface (Fig. 5(b)), reaching fluxes of \( 10^{23} \text{–} 10^{25} \, \text{ions/cm}^2/\text{s} \) in the area covered by the plasma sheath. This flux is the same as obtained with the earlier 1D version of the code [10]. In the current 2D simulation, the most probable impact energy of the bombarding ions is on the order of 25 eV, with the distribution becoming negligible above 200 eV (Fig. 5(b)). This energy range is given by the plasma sheath potential (Fig. 6(f)).

In our model, the intense ion bombardment triggers the high-flux sputtering model (Sec. 3.3.2), which releases many more neutrals than what is produced by the single-impact sputtering model (Fig. 4(b)) at these ion impact energies. Many of the sputtered neutrals are quickly ionized (Fig. 4(b)), increasing the size and density of the plasma. In addition to the ion bombardment of the cathode surface, ions are also accelerated to high speed towards the anode by waves in the electric potential, triggering sputtering there as well. Sputtering from the anode has been observed in DC experiments with small gaps [61].

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(a) Typical simulated current and voltage, as described in Sec. 4.1. The symbols are as defined in Fig. 2.

(b) Typical measured current and voltage from the DC spark experiment [59]. Plot reproduced from [60].

Fig. 3 Typical current and voltage evolution from experiment and simulation. The time intervals annotated on the plots are the fall times from 90% to 50% and 10% of the initial voltage.

(a) Flow of charged particles through the cathode.

(b) Injection and removal of neutrals.

Fig. 4 Particle fluxes due to different processes in the model as a function of time for the reference simulation described in Sec. 4.1. All traces except $I_{\text{circ}}$ are smoothed using a boxcar smoother with a 0.886 ps window for better readability.

(a) Flux as a function of time and $r$.

(b) Energy spectrum, integrated over total simulation time.

Fig. 5 Statistics for ions arriving on the cathode surface for the reference simulation described in Sec. 4.1.
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Table 1 Parameters for the presented simulations.

(a) Potential at $t = 0.8$ ns  
(b) Potential at $t = 1.0$ ns.  
(c) Potential at $t = 1.5$ ns.  
(d) Potential at $t = 2.0$ ns.  
(e) Color bar for the contour plots in (a)–(d) [V].  
(f) The electric potential as a function of $z$ at three different values of $r$ at $t = 1.5$ ns. Note the semi-logarithmic scale on the y-axis, which is linear between 0 and 10 V, then logarithmic above 10 V.

Fig. 6 The electric potential in the reference simulation described in Sec. 4.1.
Fig. 7  Density of copper, copper ions, and electrons at different stages of the arc, for the reference simulation described in Sec. 4.1.
Fig. 8  Velocity distributions and temperatures estimated from the sample variance of the distributions, shown separately for each species and vector component in the reference simulation described in Sec. 4.1. Also plotted is a Gaussian fit with the same mean, variance and normalization as the particle distributions.

Some secondary electrons are also present, but as seen in Fig. 4(a) these are outnumbered by the field emission current, and thus SEY a negligible source of electrons.

Once the enhanced sputtering sets in, the plasma quickly expands (Figs. 6(c) and 7(c)) filling the volume and expanding the sheath, which triggers emission from a rapidly increasing area on the cathode surface. As seen in Fig. 7(c) the Cu\textsuperscript{+} and e\textsuperscript{-} density now reaches 10\textsuperscript{18}–10\textsuperscript{20} cm\textsuperscript{-3}. Defining the plasma sheath footing as the region affected by the enhanced sputtering yield, the average electric field in this region is approximately 3 GV/m throughout the simulation, which is sufficient to maintain the arc. The average net current density in the region of the footing is 1 A/µm\textsuperscript{2} and the radial growth rate of the sheath footing while it is expanding is approximately 1–3 km/s. The observed number and current densities are consistent with the experimental data reported in [62]. Further, Fig. 8(a) shows that the velocity distributions are non-Gaussian, as expected for a collisionless plasma. This is especially true for the z-components for the charged particles, due to the electric field.
The rise in the gap current continues until the voltage $V_{\text{gap}}$ collapses to a small value, at which point the current stops rising and then rapidly drops to the circuit limited value $I_{\text{circ}}$, such that $I_{\text{circ}} \approx I_{\text{lim}} = U/R$ (Figs. 6(d) and 7(d)). When this happens, the area covered by the arc footing shrinks as well, such that the current density stays constant. Note that in Fig. 8(b) the velocity distributions are more Gaussian than in Fig. 8(a) but there is still variation between species and velocity components. At this point, the long-term burning of the arc can only be maintained with the aid of an external energy supply. However, the long-term burning cannot be simulated with our present model, as further species of higher ion charge states would need to be included [33].

4.2 Effects of the surface model parameters on the transition into the volume-defined phase

In order to see the effects of the high-flux sputtering model and the evaporation model, we ran a small scan of the relevant parameters. Additionally, we also ran one simulation with $\beta_{\text{flat}} = 1.0$. The resulting current and voltage curves from these simulations are shown in Fig. 9.

![Current and voltage evolution for different surface model parameters](image)

(a) Voltage, dashed lines indicate 90%, 50% and 10% of the initial voltage.

(b) Current, $I_{\text{gap}}$ plotted as solid line, $I_{\text{circ}}$ as dashed line. The flat spot on $j_{\text{enhanced}} = 10^{24}$ ions/cm$^2$/s is due to an intermittent drop-out of storage of output data.

**Fig. 9** Current and voltage evolution for different surface model parameters, as discussed in Sec. 4.2. The legend indicates which parameter was changed from the reference value and the new value.

The main purpose of these simulations was to look for thresholds where the transition into the volume-defined phase is no longer possible, in order to understand what conditions are necessary for the arc to spread. For the high-flux sputtering model, it was found that both increasing the threshold $j_{\text{enhanced}}$ to $10^{26}$ ions/cm$^2$/s and setting $Y_{\text{enhanced}} = 0$ resulted in that the transition to the volume-defined phase never happened, at least not within the time scales covered by the simulation. In other words, a sputtering process providing increased sputtering yield compared to the single-impact model is necessary to enter the volume-defined phase of the arcing, as the average sputtering yield from the single-impact model ($\approx 0.11 < 1.0$) is too low to maintain and expand the arc.

When increasing $Y_{\text{enhanced}}$ from 1 to 2, the results were quite similar to the reference simulation, except for that the current $I_{\text{gap}}$ rose slightly faster and the number of neutrals created was higher. Note that while the number of injected neutrals from the high-flux sputtering and evaporation in the reference simulation (Fig. 8(b)) are by chance almost identical, this is no longer the case after changing $Y_{\text{enhanced}}$.

The roughness of the “flat” cathode surface does not play an important role at the levels tested, as decreasing $\beta_{\text{flat}} = 2$ to $\beta_{\text{flat}} = 1$ was still sufficient to enter the volume-defined phase, with the main difference being that $I_{\text{gap}}$ rose slightly slower.

When the evaporation ratio $r_{\text{Cu/e}}$ was lowered from 0.015 to 0.01, ions were not created fast enough, and the space charge screening was never overcome. Thus no discharge was created within the 3 ns for which the simulation was allowed to run, and there were no indications that one was about to ignite. However, one should be careful when interpreting this threshold, as the simple evaporation model used
in these simulations is mainly intended as a method for providing some initial gas which is necessary to start the arc. Especially, the injection energy is intentionally elevated, as mentioned in Sec. 3.4.

In summary, we have shown that under suitable circumstances the cathode spot can spread and, due to the plasma sheath, enhance the field in a large area around the original field emitter. As mentioned before, we aim only at describing the build-up of the arc, and hence, we restrict our model to a single field emitter in a cylindrically symmetric system and a homogeneous surface around it. In reality, the surface is never perfectly homogeneous and smaller field emitters on the “flat” surface would further enhance the field, breaking the symmetry and creating further footings of the arc.

4.3 The effects of the circuit parameters on the fall time of the gap voltage

Using the reference simulation parameters as a starting point, we varied the circuit parameters $C_{\text{gap}}$ and $R$ in order to study the effect on the voltage fall times $t_{90\%/50\%}$ and $t_{90\%/10\%}$. These quantities are defined as the time between the moments when $V_{\text{gap}}$ crosses 90% of $U$ to when it crosses 50% or 10% of $U$. Also studied was the peak gap current $I_{\text{gap}}$ and circuit limited current $I_{\text{lim}}$. The results from this study are shown in Tab. 2 and Fig. 10. Most of these simulations were not ran until the current became circuit-limited, but interrupted earlier as they were using large amounts of computing time. In these cases, the maximally reached current $I_{\text{gap}}$ is therefore smaller than what it would have been if the simulations were allowed to run to completion.

**Table 2** Circuit parameters and simulation results as discussed in Sec. 4.3.

<table>
<thead>
<tr>
<th>$C_{\text{gap}}$ [pF]</th>
<th>$R$ [Ω]</th>
<th>$t_{90%/50%}$ [ns]</th>
<th>$t_{90%/10%}$ [ns]</th>
<th>$I_{\text{gap}}$ [A]</th>
<th>$I_{\text{lim}}$ [A]</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1000</td>
<td>0.27</td>
<td>0.42</td>
<td>6.8</td>
<td>1.74</td>
<td>Reference sim. (Sec. 4.1)</td>
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<td>0.0</td>
<td>100</td>
<td>0.45</td>
<td>-</td>
<td>&gt;13.2</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>100</td>
<td>0.40</td>
<td>-</td>
<td>&gt;18.5</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>500</td>
<td>0.28</td>
<td>0.50</td>
<td>7.1</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>5000</td>
<td>0.26</td>
<td>0.40</td>
<td>6.2</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>2.0</td>
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<td>-</td>
<td>&gt;10.1</td>
<td>-</td>
<td></td>
</tr>
<tr>
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<td>5000</td>
<td>0.21</td>
<td>0.38</td>
<td>2.6</td>
<td>0.35</td>
<td></td>
</tr>
</tbody>
</table>

(a) Voltage, dashed lines indicate 90%, 50% and 10% of initial voltage, used to calculate $t_{90\%/50\%}$ and $t_{90\%/10\%}$.

(b) Current, $I_{\text{gap}}$ plotted as solid line, $I_{\text{circ}}$ as dashed line.

**Fig. 10** Current and voltage evolution for different circuit model parameters, as discussed in Sec. 4.3. The legend indicates which parameter was changed from the reference value and the new value.

In addition to the simulations listed in Tab. 2 we also ran some simulations with $U = 870$ V ($E_{z} = 145$ MV/m, $E_{\text{loc}} = 5$ GV/m) and $U = 5700$ V ($E_{z} = 950$ MV/m, $E_{\text{loc}} = 33$ GV/m). In these simulations, the circuit parameters were either $R \rightarrow \infty$ (no external supply), or $C_{\text{gap}} = 0$ and several different $R$. For the low-voltage simulations, no ionization avalanche occurred within the 6 ns for which the simulations
were allowed to run, and the current stayed constant throughout the entire run. The high-voltage simulations were similar to the other spreading simulations presented in this paper, the main exception being that the time before the ionization avalanche started was only around 0.1 ns. The results from both the high- and low voltage simulations are in agreement with the experimental observation that breakdowns only occur above a local field of approximately 10 GV/m.

From the simulations shown in Tab. 2 and Fig. 10 we note that the voltage fall times and peak gap currents have some dependency on the circuit parameters. For the gap capacitance $C_{\text{gap}}$, this is due to that a larger capacitance stores a larger amount of charges, allowing the gap current to grow for a longer time, overshooting the circuit-limited value, before the surface charge is used up and the gap current falls to the circuit-limited value $I_{\text{lim}}$.

As also observed in the DC spark experiment, in our simulations the dependence of the fall times on $C_{\text{gap}}$ is relatively weak [59]. While not tested in the experiments, we observed that the dependence on the circuit resistance $R$ is stronger, with the smaller resistance values yielding longer fall times and higher peak currents. This is due to the smaller resistance values allowing more current to flow from the external supply to the gap, putting less load on the gap capacitance and hence its charge is drained slower.

Comparing the current- and voltage curves to what is seen in the DC spark experiment (Fig. 3(b)), we see that the shapes and fall times are matching reasonably well. The remaining differences can be explained by a combination of the lower resistance and higher gap capacitance in the experiment, and uncertainties in the surface model. Limitations in how quickly the experimental circuit can deliver current and how fast rise-times can be measured are also likely to play a role. Especially, the smallest voltage fall time currently measurable in the DC spark experiment is on the order of 5 ns, as estimated from the stated bandwidth of the voltage probe [59], which means experimentally the rise times predicted by the simulation for different circuit parameters can currently not be distinguished.

5 Conclusions

In this paper, we have presented results from a new simulation tool for studying the plasma build-up in a copper vacuum arc, showing how the properties of the surface and the circuit supplying the spark gap affect the plasma during the transient. The predicted current and plasma densities are consistent with previously reported experimental data. Furthermore, the time scales of the transient are similar to what was measured in the DC spark system.

We have shown that plasma initiation can occur when sufficient field emission and neutral evaporation is provided, and that surface physics processes at the cathode play a crucial role. During the initiation, the simulated discharge goes through three phases: field emission, breakdown, and volume-defined arc discharge. We also demonstrated how the cathode spot starts spreading after entering the volume-defined phase.

The tool presented opens the possibility for further studies of how the plasma interacts with the surface and external circuit, and how this affects the initiation and development of vacuum arcs. This is useful for guiding experiments, for developing new surface models, as well as for understanding the field parameters necessary to initiate a vacuum arc in high-gradient RF accelerating structures.

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