Significance of different physical interactions in initiation of vacuum arcing

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Stages of vacuum arc plasma formation

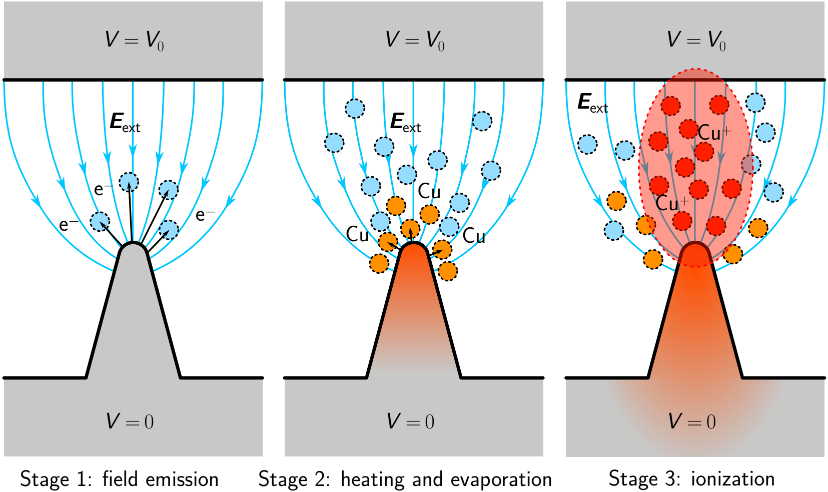


Figure 1: Initial stages of plasma formation.

Electric field, emission, heating

- Assume field emitter on surface $\rightarrow$ field enhancement $\rightarrow$ field emission of electrons
- Two main heating effects: Nottingham heating (NH) on the surface and Joule (resistive) heating (JH) in the bulk
- Evaporation of neutrals causes cooling (VH)
- Particle bombardment deposits additional heat on surface as plasma starts forming (BH)

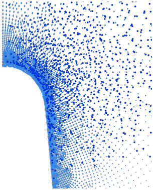


Figure 2: Field and electrons.

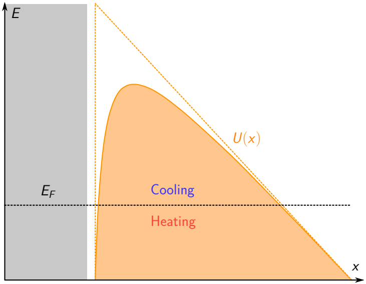


Figure 3: Electron $\langle \Delta E \rangle \rightarrow$ cooling/heating. Figure adapted from [1].

[1] A. Kyritsakis. Electron emission calculations beyond the classical equations: finite size, space charge and thermal effects in sharp emitters. IVNC 2021.

Vacuum arc simulations

- Previous ArcPIC [2] code focused on plasma simulation, no heating effects
- FEMOCS (Finite Elements on Crystal Surfaces) code [3]
  - Concurrent, multi-scale, multi-physics
  - Finite element method (FEM), particle-in-cell method (PIC), connects to molecular dynamics (MD)
  - Combines electric field and heating calculations
  - Emission calculated using GETELEC code
- Current work: combine emission and heating calculations with plasma simulation
  - Significance of different interactions
  - Influence of surface-plasma interactions

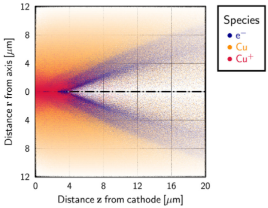


Figure 4: ArcPIC [2].

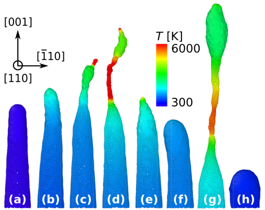


Figure 5: FEMOCS [3].

[2] H. Timko et al. From field emission to vacuum arc ignition: A new tool for simulating copper vacuum arcs. Contributions to Plasma Physics, 2015.
[3] M. Veske et al. Dynamic coupling between particle-in-cell and atomistic simulations. Phys. Rev E., 2020.

Field solution using finite element method (FEM)

- Solve PDEs of system using finite element method
  - Poisson's equation
    $\nabla \cdot (\varepsilon_0 \nabla \phi) = -\rho$ in vacuum
    $\rightarrow$ electric field
  - Continuity equation
    $\nabla \cdot (\sigma \nabla \phi) = 0$ in bulk
    $\rightarrow$ current density
  - Heat equation
    $\nabla \cdot (\kappa \nabla T) + P_J = C_v \partial_t T$ in bulk
    $\rightarrow$ temperature

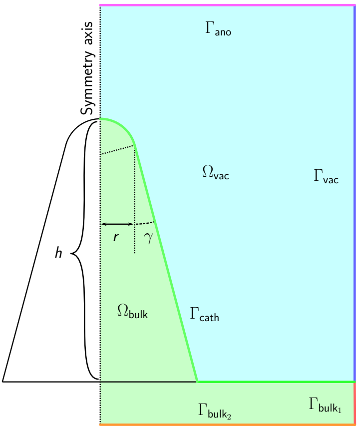


Figure 6: Domains in simulation, vacuum (blue) and bulk Cu (green).

Particle-in-cell (PIC) simulation of plasma

- Particles injected to system at cathode surface (emitted electrons, evaporated neutrals)
- Large number of particles e.g. electrons can be modelled as superparticles (SPs)

1. Calculate motion of particles in cell (leapfrog method)
2. Calculate electric field for mesh (solve Poisson's equation using FEM)
3. Do Monte Carlo collisions between particles within each cell [4]

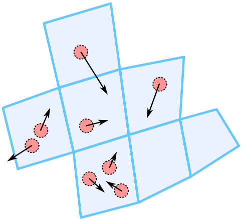


Figure 7: SPs in mesh.

[4] T. Takizuka and H. Abe. A binary collision model for plasma simulation with a particle code. Journal of Computational Physics, 1977.

Collision types

1. Elastic collisions
   1. Cu + e^- $\rightarrow$ Cu + e^-
   2. Cu + Cu $\rightarrow$ Cu + Cu
2. Coulomb collisions for all charged particles
3. Impact ionization [5]
   1. Neutrals: Cu + e^- $\rightarrow$ Cu^{n+} + (n + 1) e^-
   2. Ions: Cu^{i+} + e^- $\rightarrow$ $Cu^{(i+n)+}$ + (n + 1) e^-
4. Charge exchange [5]: Cu + Cu^+ $\rightarrow$ Cu^+ + Cu
5. Radiative recombination: Cu^+ + e^- $\rightarrow$ Cu + (γ)

Collision probability [6]

Collision takes place when $R \sim U(0,1) < P$,

$$P = 1 - \exp\left(-un\sigma(E)\Delta t\right), \qquad (1)$$

where n is the lower number density of the two colliding particle types, σ is the cross section and Δt is time step.

[5] K. Matyash. Kinetic modeling of multi-component edge plasmas. PhD thesis, University of Greifswald, 2003.

[6] V. Vahedi and M. Surendra. A Monte Carlo collision model for the particle-in-cell method: applications to argon and oxygen discharges. Computer Physics Communications, 1995.

Field ionization

- Evaporated neutrals ionized directly by tunneling [6]
- Expected to dominate ionization processes when field is high
- Ammosov–Delone–Krainov (ADK) model

Probability of direct field ionization [7]

$$P = \frac{1.52 \times 4^n \xi}{n\,\Gamma(2n)\ \mathrm{fs}} \left(20.5 \frac{\xi^{3/2}}{E}\right)^{2n-1} \exp\left(-6.83 \frac{\xi^{3/2}}{E}\right), \tag{2}$$

where $n = 3.69 z \xi^{-1/2}$ and P is probability (1 / fs), ξ is the potential of ionization (eV), E is the electric field (GV / m) and z is charge after ionization.

[6] D. Bruhwiler et al. Particle-in-cell simulations of tunneling ionization effects in plasma-based accelerators. Physics of Plasmas, 2003.

[7] S. Calatroni. Direct field ionization. In 8th International Workshop on Mechanisms of Vacuum Arcs, 2019.

Ion bombardment

- Ions are accelerated by the electric field
- Two effects: sputtering and bombardment heating
- Ions can cause neutrals to be sputtered from the surface depending on energy $\rightarrow$ sputtering yield
- Remaining energy is deposited as heat into the surface

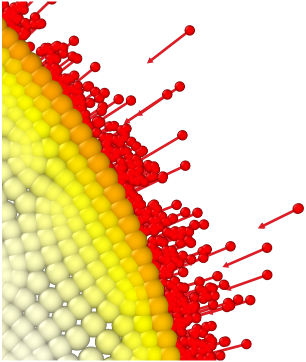


Figure 8: Cu^{+} ions (red) bombarding cathode surface.

Circuit model

- In the real circuit, we have impedance
- Circuit model with resistor $I_{\text{circ}} = \frac{U - V_{\text{gap}}}{R}$ and capacitor
- Capacitance across gap with $C_{\text{gap}} = Q_{\text{gap}} / V_{\text{gap}}$ and $I_{\text{cap}} = I_{\text{gap}} - I_{\text{circ}}$
- Calculate gap current I_{gap} from Shockley-Ramo theorem
- Ongoing work: model impedance on entire cathode surface, influence of power coupling

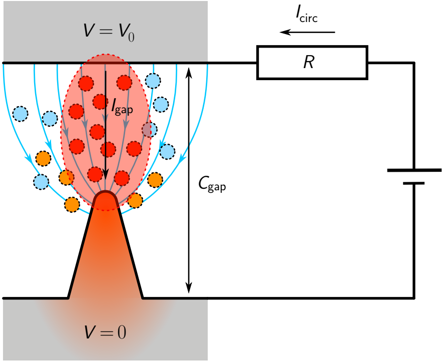


Figure 9: Vacuum arc circuit.

Present simulation model

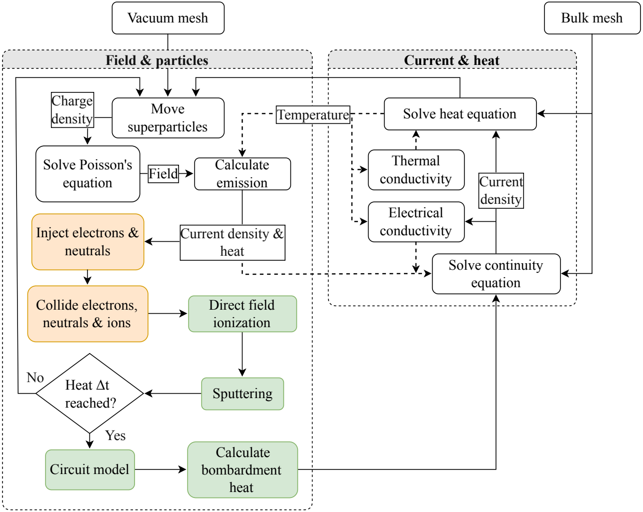
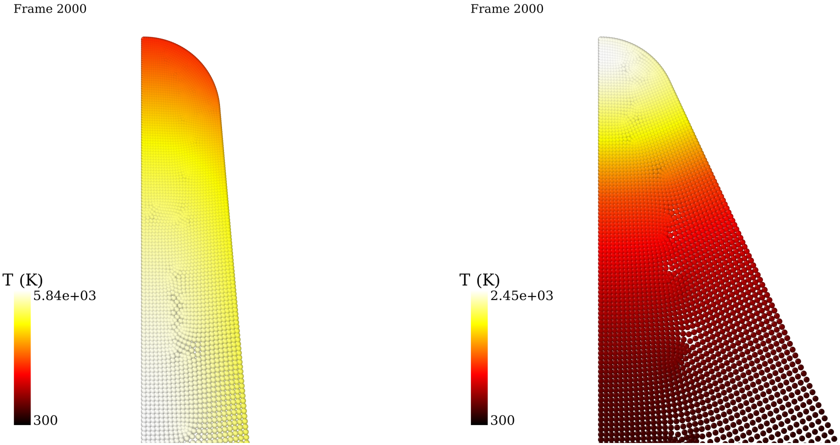


Figure 10: Flowchart of present model with PIC additions, excluding MD.

Heating of static nanotip

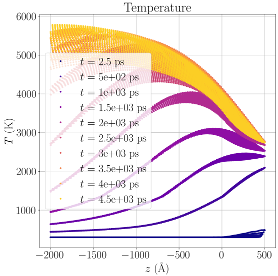


(a) Tip with $\gamma = 5°$.

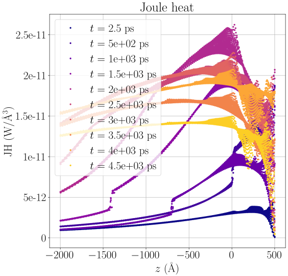
(b) Tip with $\gamma = 25°$.

Figure 11: Temperature distributions, $F_{\rm loc} = 10$ GV/m, $t = 5$ ns, JH+NH.

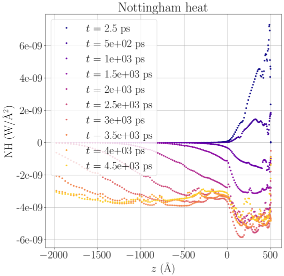
Heat sources



(a) Bulk temperature.



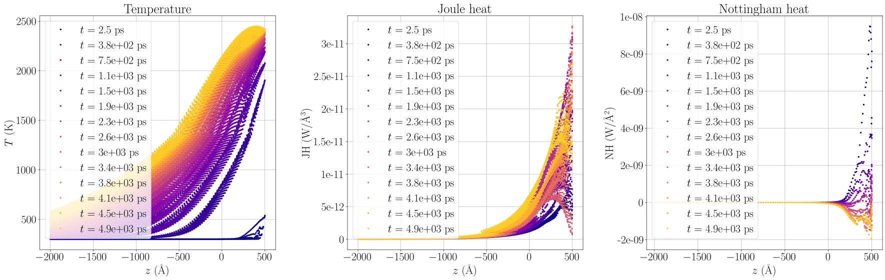
(b) Bulk Joule heat.



(c) Surface Nottingham heat.

Figure 12: Temperature/heat distributions for $\gamma = 5^{\circ}$.

Heat sources



(a) Bulk temperature. (b) Bulk Joule heat. (c) Surface Nottingham heat.

Figure 13: Temperature/heat distributions for $\gamma = 25^\circ$.

Heat sources

- Total Nottingham heat changes from heating to cooling
- Nottingham heat more significant at the start
- Overall, Joule heating dominates at later stages

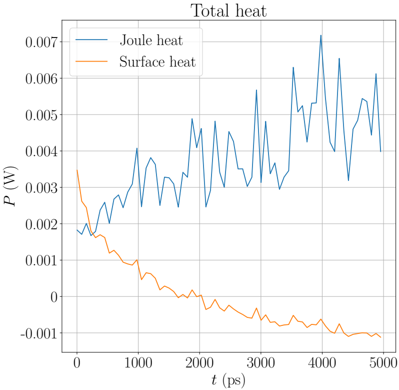


Figure 14: Total heat in bulk for $\gamma = 25^\circ$.

Simulation 1

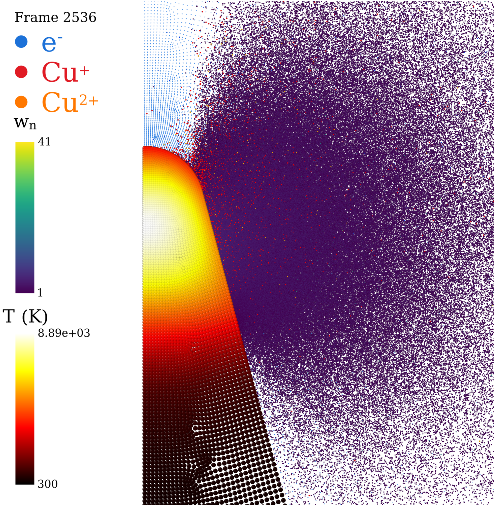


Figure 15: Nanotip $r = 50$ nm, $h = 50r$, $F_{\text{loc}} = 13$ GV/m.

Simulation 2

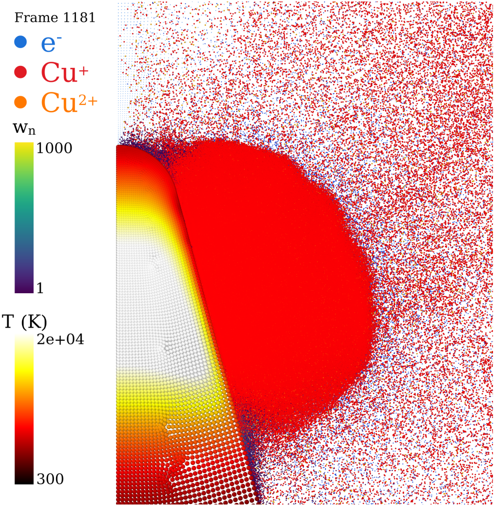
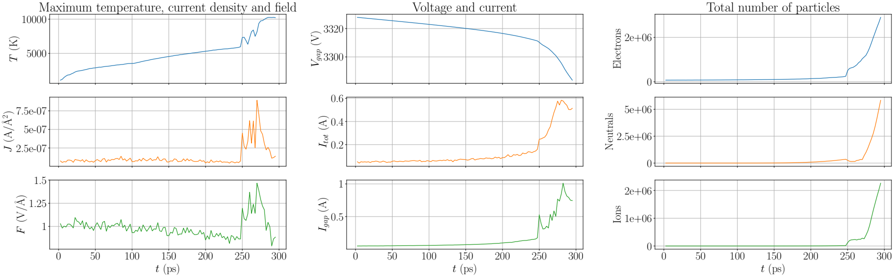


Figure 16: Nanotip $r = 50$ nm, $h = 50r$, $F_{\text{loc}} = 15$ GV/m.

Simulation 2

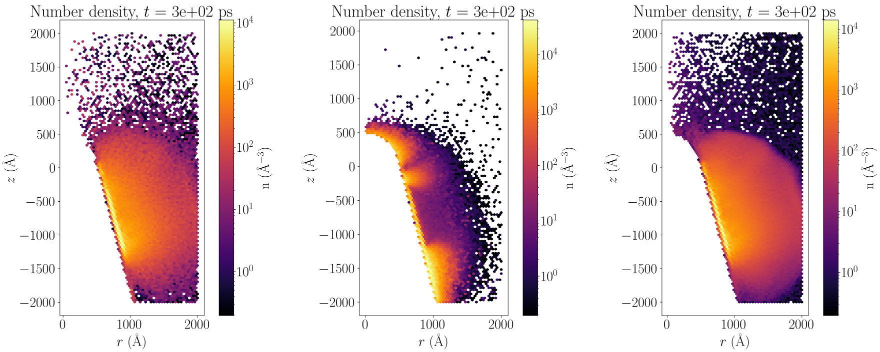
- A runaway process occurs when field is sufficiently high



(a) Surface maximums. (b) Voltage and current. (c) Number of particles.

Figure 17: State of $F_{\mathrm{loc}} = 15$ GV/m system.

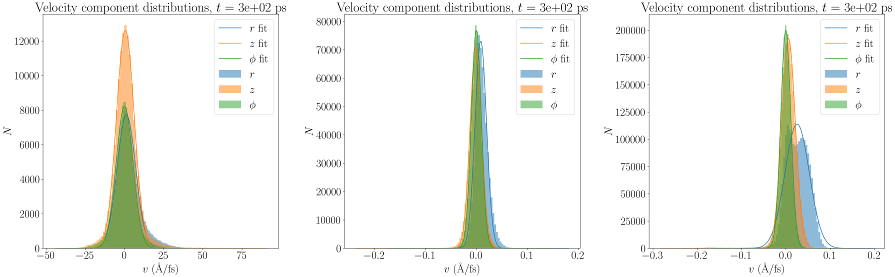
Plasma formation



(a) Electrons. (b) Neutrals. (c) Cu^{+} ions.

Figure 18: Number density distributions at $F_{\mathrm{loc}} = 15$ GV/m.

Plasma formation

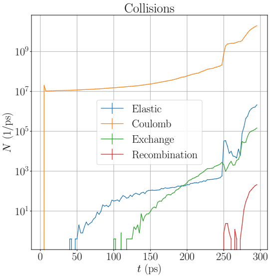


(a) Electrons. (b) Neutrals. (c) Cu^+ ions.

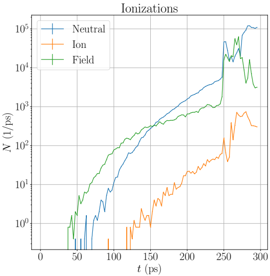
Figure 19: Velocity distributions at $F_{\text{loc}} = 15$ GV/m.

Significance of interactions

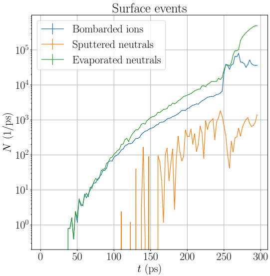
- Field ionization more significant at early stages
- Few sputtered neutrals vs. evaporation, bombardment mostly heat



(a) Collisions.



(b) Ionizations.



(c) Surface interactions.

Figure 20: Particle interaction events.

Surface heat sources

- Nottingham heat much more significant than other heat sources
- Evaporative cooling and bombardment heating contribute up to approximately 10% of heating
- Net cooling of cathode surface

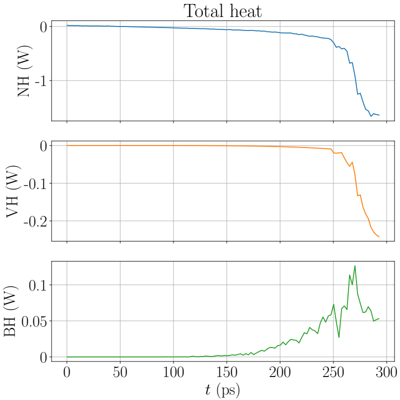


Figure 21: Total heat on the surface for $F_{\text{loc}} = 15$ GV/m.

Conclusions

- Thermal runaway and plasma formation can be reached by simulating a static nanotip
- Heating dynamics is influenced by multiple factors, namely the interplay between Joule and Nottingham heating, as well as tip geometry
- Field ionization is more significant than impact ionization at the start of plasma formation, while at a later stage the reverse is true
- Plasma-surface interactions can significantly impact vacuum arc initiation
- Ongoing work:
  - Cathode surface modification, MD-plasma interaction
  - Circuit power coupling

Upcoming publication: R. Koitermaa, A. Kyritsakis, T. Tiirats, V. Zadin, and F. Djurabekova. Simulating vacuum arc initiation by coupling emission, heating and plasma processes. 2023.

Thank you!