Concurrently coupled particle-in-cell, emission, and heating simulations of vacuum arc plasma initiation

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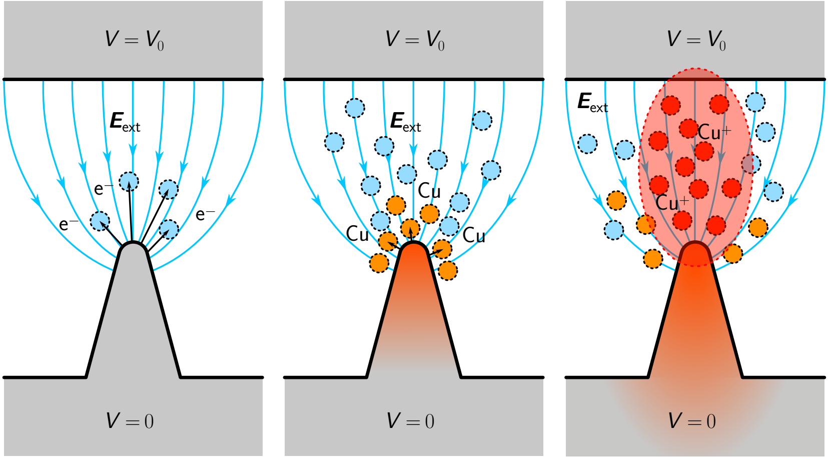
Stages of vacuum arc plasma formation



Stage 1: field emission Stage 2: heating and evaporation Stage 3: ionization

Figure 1: Initial stages of plasma formation.

Vacuum arc simulations

- Previous ArcPIC [1] code focused on plasma simulation
- FEMOCS (Finite Elements on Crystal Surfaces) code [2]
  - Concurrent, multi-scale, multi-physics
  - Finite element method (FEM), particle-in-cell method (PIC), connects to molecular dynamics (MD)
  - Combines electric field and heating
  - Emission calculated using GETELEC
- Current work: combine emission and heating calculations with plasma simulation
  - Significance of different interactions
  - Influence of surface-plasma interactions

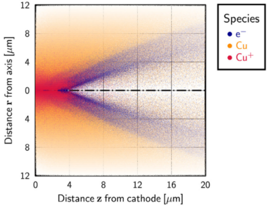


Figure 2: ArcPIC [1].

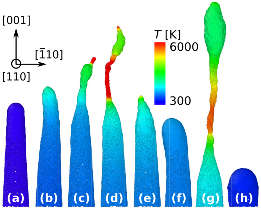


Figure 3: FEMOCS [2].

[1] H. Timko et al. From field emission to vacuum arc ignition: A new tool for simulating copper vacuum arcs. Contributions to Plasma Physics, 2015.

[2] 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

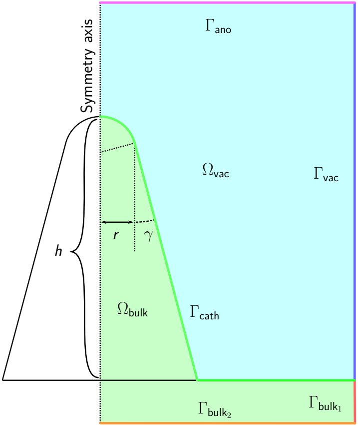


Figure 4: Domains in simulation, vacuum (blue) and bulk Cu (green).

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 [3]

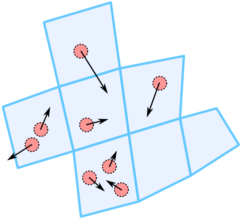


Figure 5: SPs in mesh.

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

Collision probability [5]

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

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

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

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

[5] 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.

Simulation model additions

1. Plasma simulation
2. Field ionization (significant ionization mechanism [6])
3. Bombardment effects (heating, sputtering)
4. Circuit model (under development, T. Tiirats)

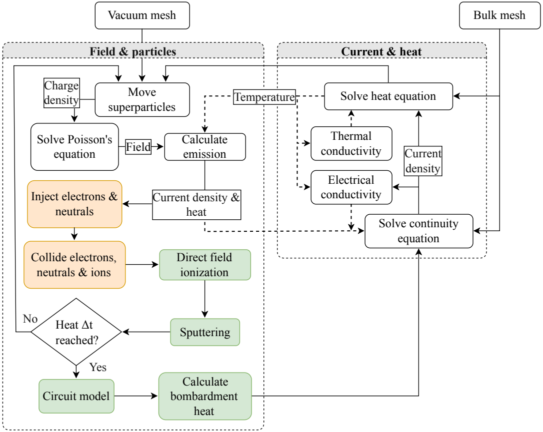


Figure 6: Flowchart of present model with PIC additions, excluding MD.

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

Simulation (15 GV/m)

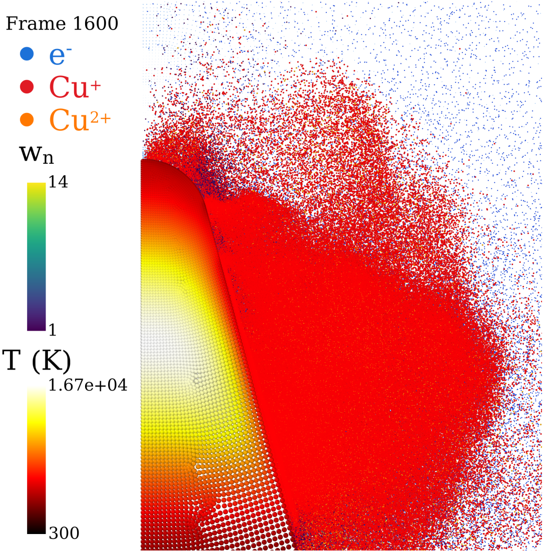
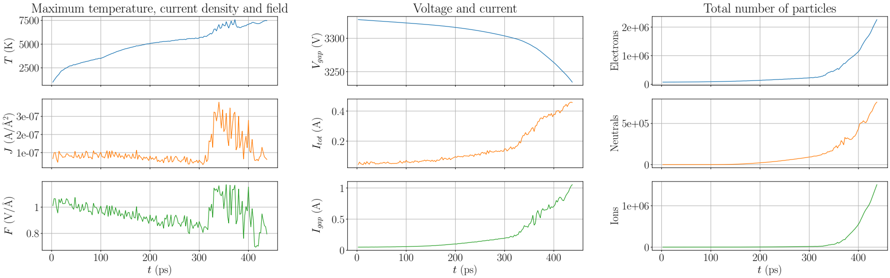


Figure 7: Nanotip $r = 50$ nm, $h = 50r$, $F_{\text{loc}} = 15$ GV/m.

Simulation (15 GV/m)

- A runaway process occurs when field is sufficiently high



(a) Surface maximums.

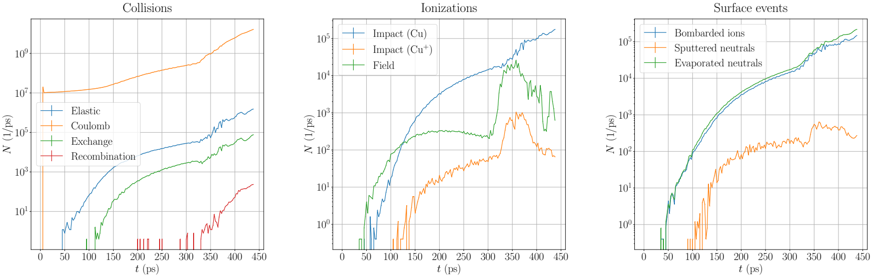
(b) Voltage and current.

(c) Number of particles.

Figure 8: State of $F_{\text{loc}} = 15$ GV/m system.

Significance of interactions

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



(a) Collisions.

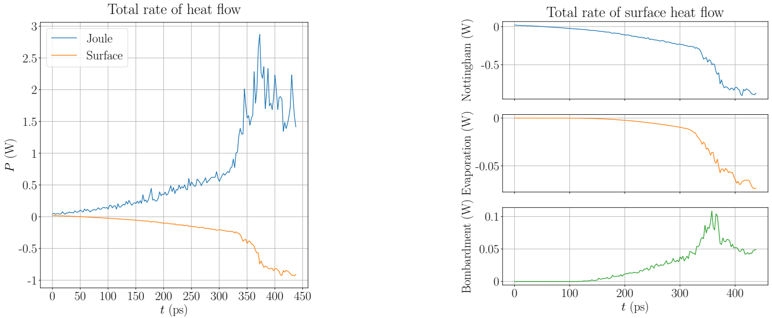
(b) Ionizations.

(c) Surface interactions.

Figure 9: Particle interaction events.

Heat sources

- Bulk: Joule heat most significant
- Surface: Nottingham heat much more significant than other heat sources, evaporative cooling and bombardment heating contribute up to 10% of total
- Net heating of bulk and cooling of cathode surface



(a) Bulk.

(b) Surface.

Figure 10: Total heat for $F_{\text{loc}} = 15$ GV/m.

Current work: molecular dynamics coupling

- Cathode modification requires molecular dynamics simulation
- First step: plasma simulation also works in 3D
- Second step: MD cathode modification + PIC plasma simulation
- TODO: particle exchange between PIC and MD

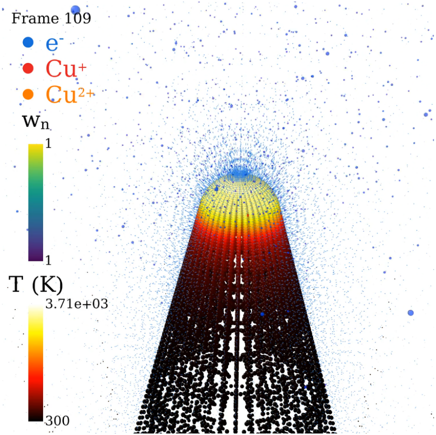


Figure 11: Plasma simulation in 3D.

Current work: molecular dynamics coupling

1. Create FEM mesh based on atom positions
2. Run FEM + PIC
3. FEM → MD atom forces + velocities
4. Run MD

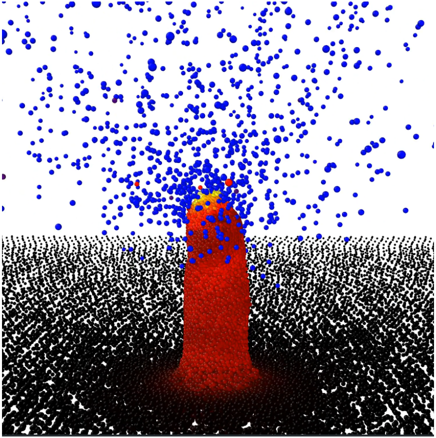


Figure 12: Plasma simulation with MD surface modification (FEM mesh).

Conclusions

- Thermal runaway and plasma formation can be reached by simulating a static nanotip
- Plasma-surface interactions can significantly impact vacuum arc initiation
- Field ionization is more significant than impact ionization at the start of plasma formation, while at a later stage the reverse is true
- Ongoing work:
  - Cathode surface modification, MD-plasma interaction
  - Circuit power coupling (Tauno Tiirats)

Preprint available: R. Koitermaa, A. Kyritsakis, T. Tiirats, V. Zadin, and F. Djurabekova. Simulating vacuum arc initiation by coupling emission, heating and plasma processes. arXiv:2402.08404 [physics.plasm-ph]

Thank you!