Unipolar Plasma Model of RF Breakdown

Z. Insepov, J. Norem

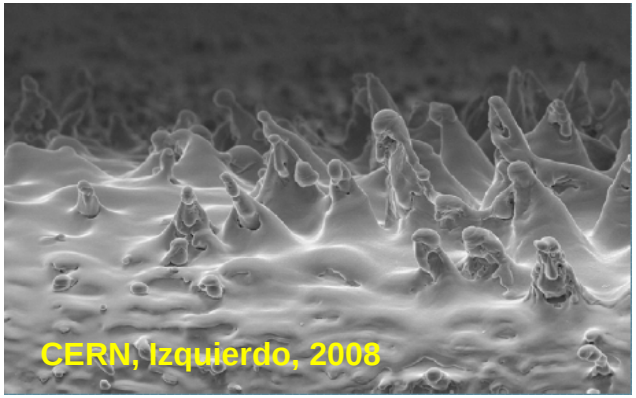
1) Purdue University, 2) Nanosynergy Inc

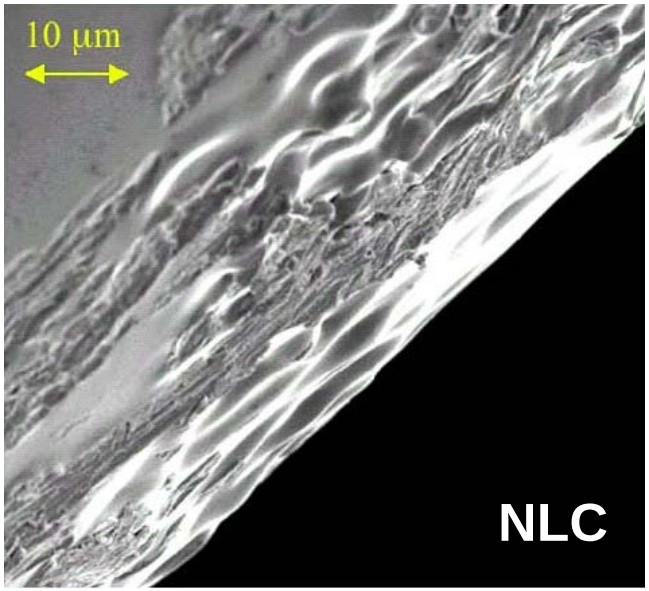
Outline

- Motivation - RF breakdown in cavities
- Calculation of electric field for real surfaces
- Experimental enhancement factor for dark current
- Cluster field evaporation in high electric field
- Unipolar (Schwirzke) plasma model development
- Surface sputtering by ions
- Atomistic model of non-Debye plasma
- Plasma model of RF BD
- Conclusions

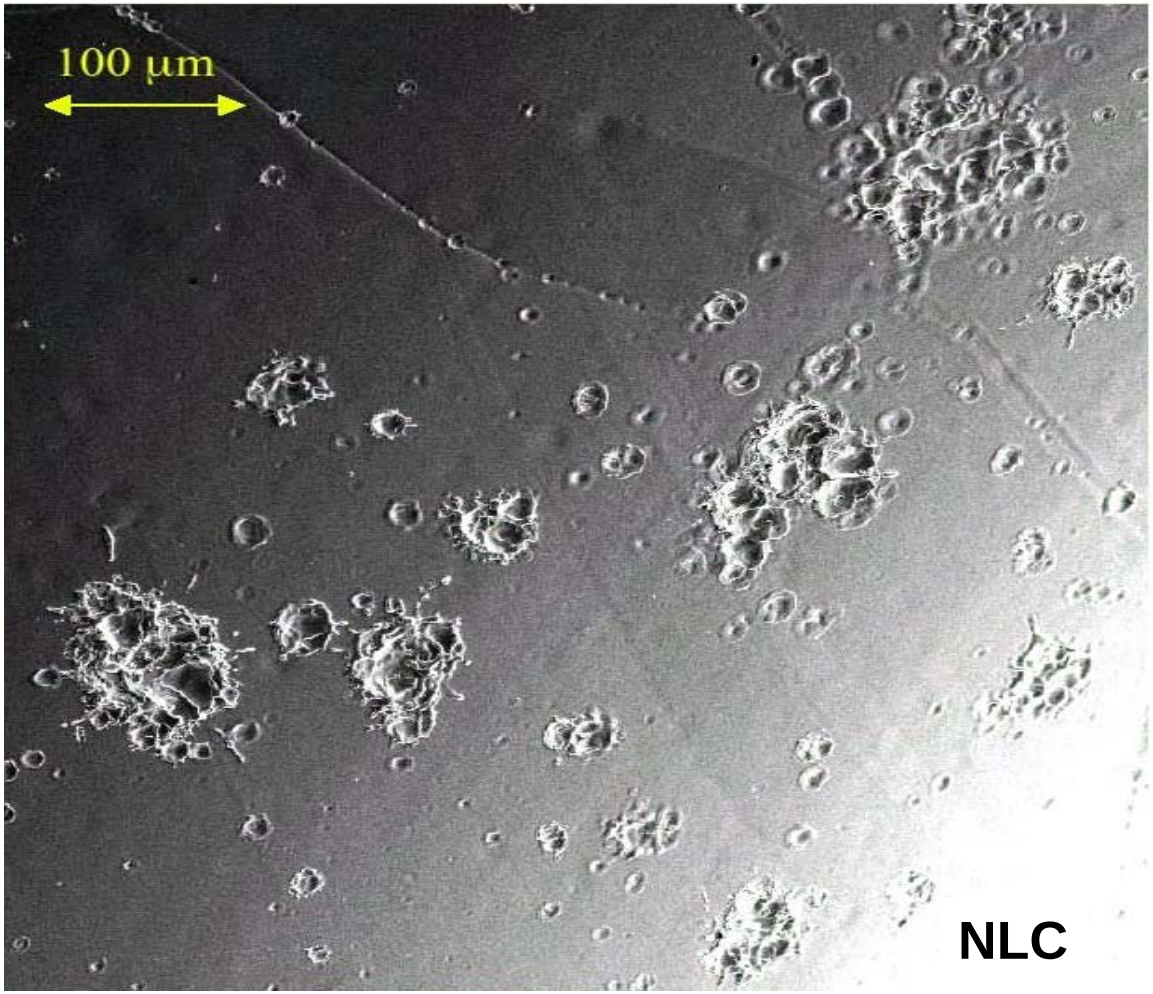
RF Breakdown examples

Severe damage





Moderate damage

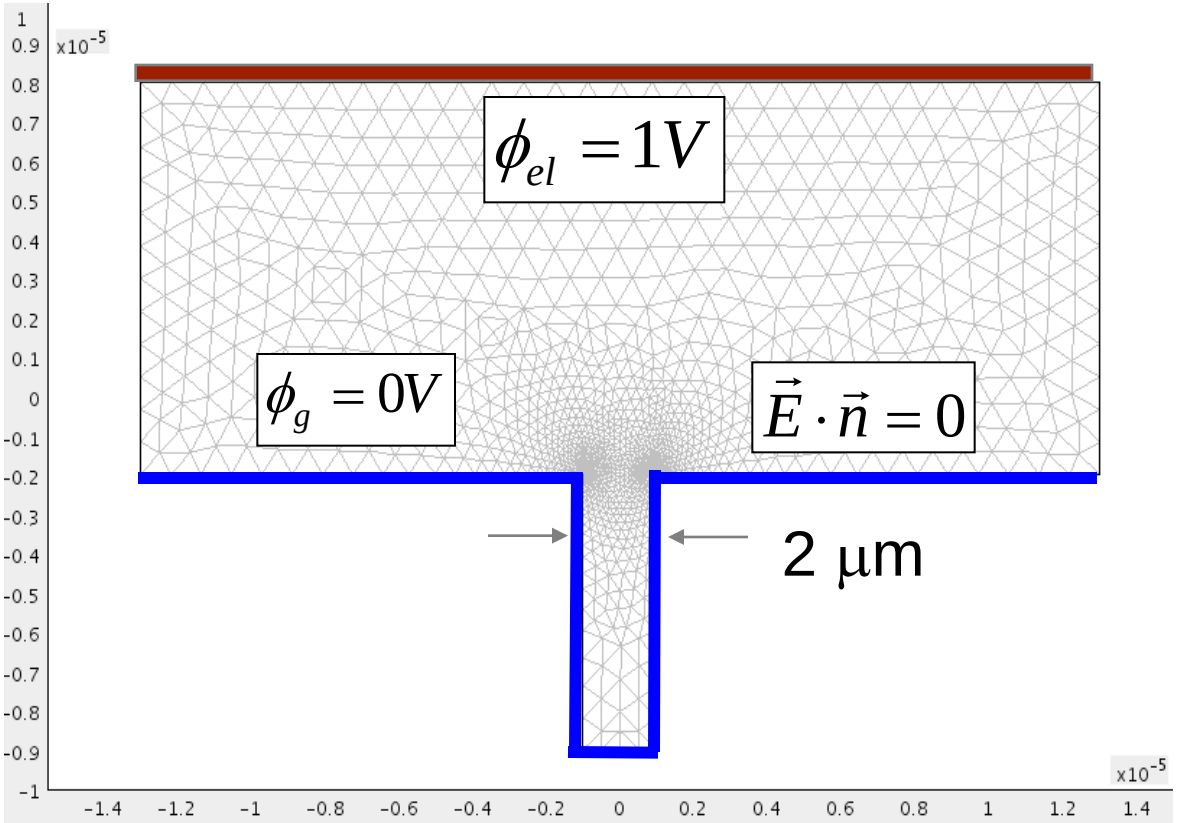


[From the 2001 Report on the Next Linear Collider]

Calculation of electric field for real surfaces

FE multi-physics simulation

- **Comsol simulation : Solving Laplace's equation for arbitrary geometry**



$$\Delta\phi = 0$$

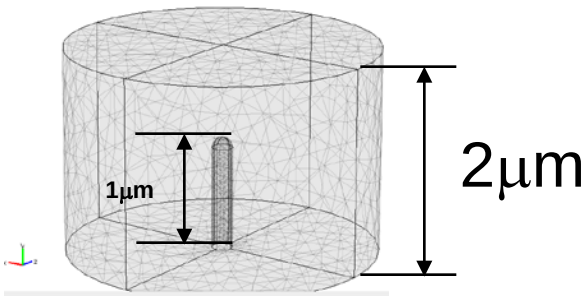
$$\vec{E} \cdot \vec{n} = 0$$

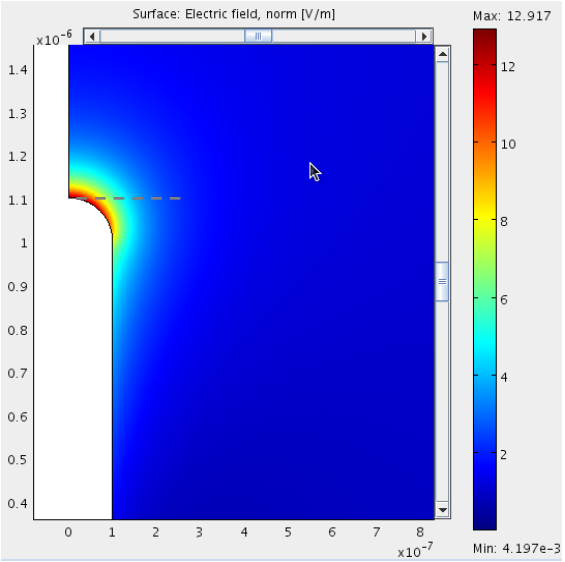
$$\phi_g = 0V$$

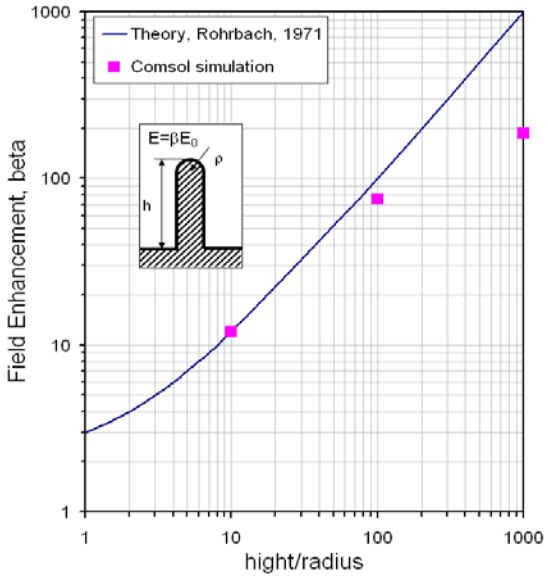
$$\phi_{el} = 1V$$

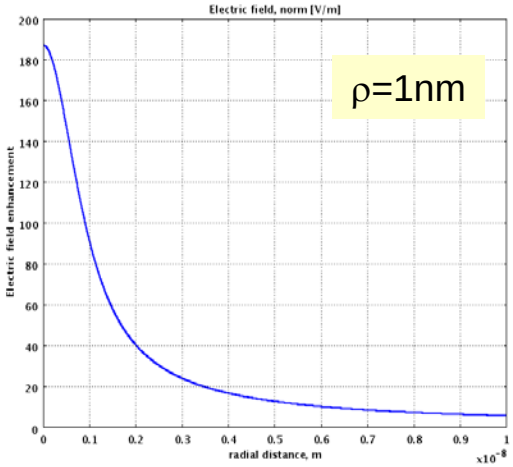
Field Enhancement by tips

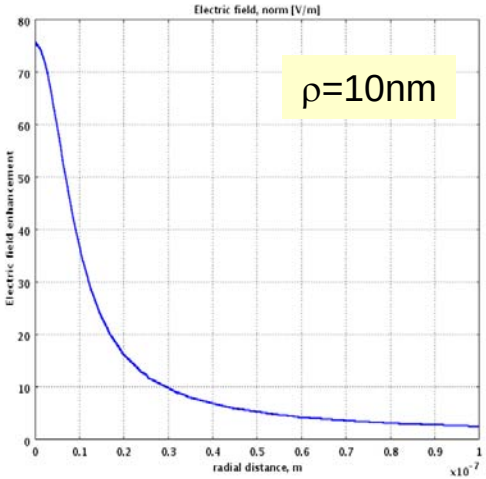
- **Comsol simulation vs analytical theory of field enhancement**

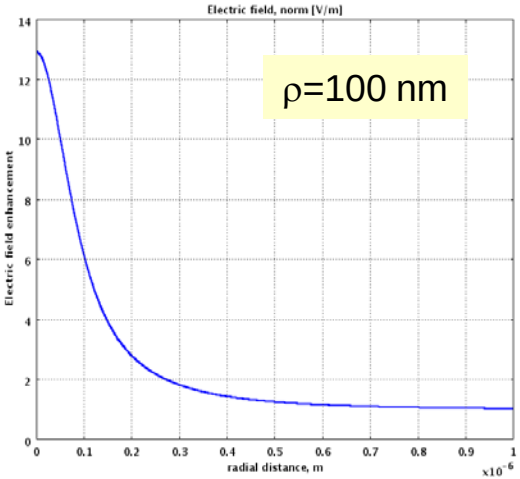






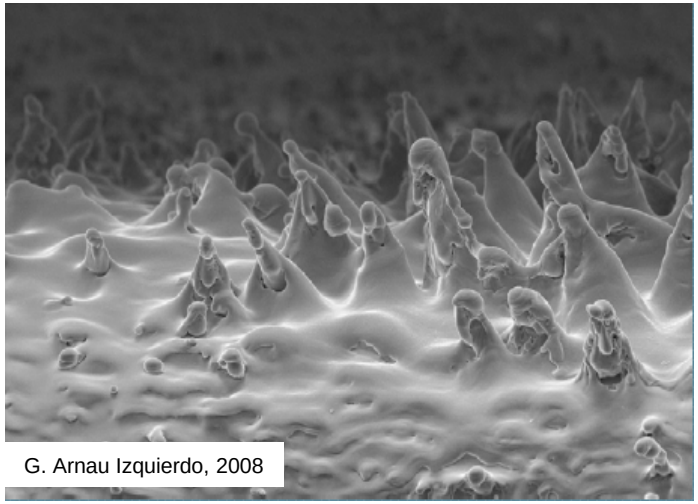


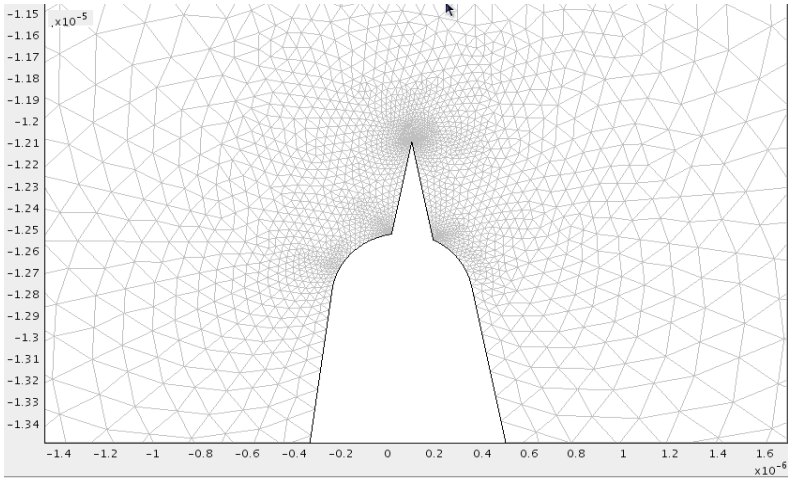


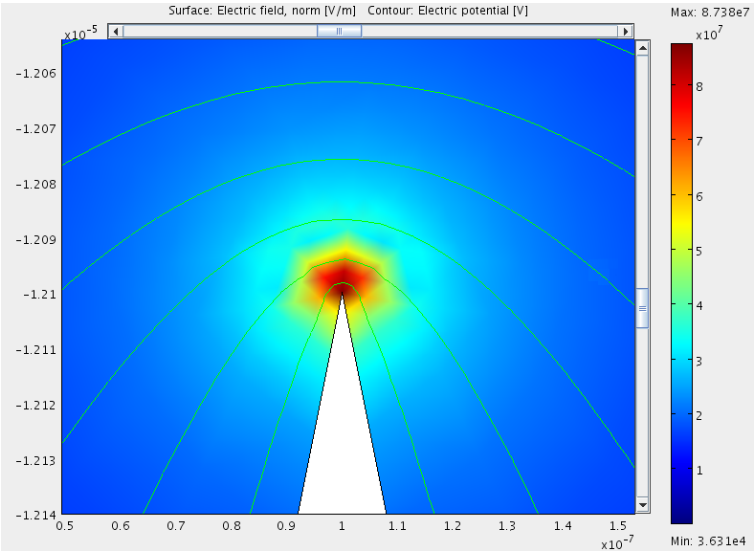


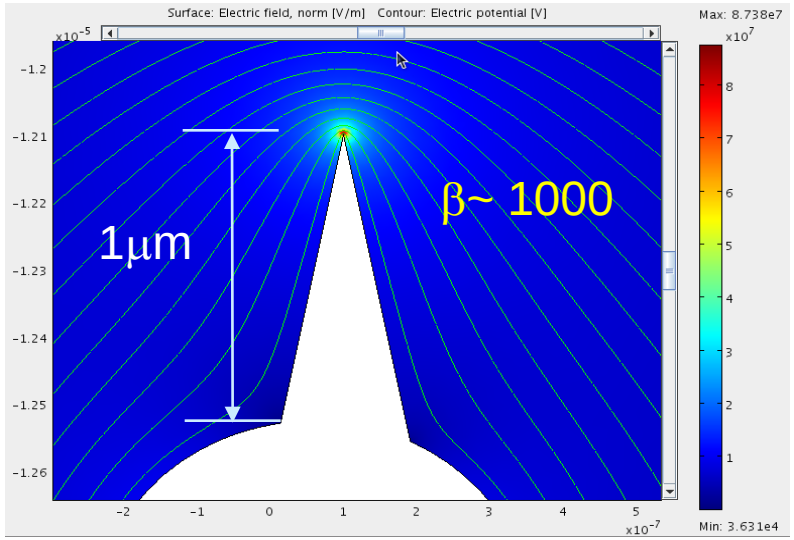
Field Enhancement by cones

- **Comsol simulation of field enhancement at sharp cones**



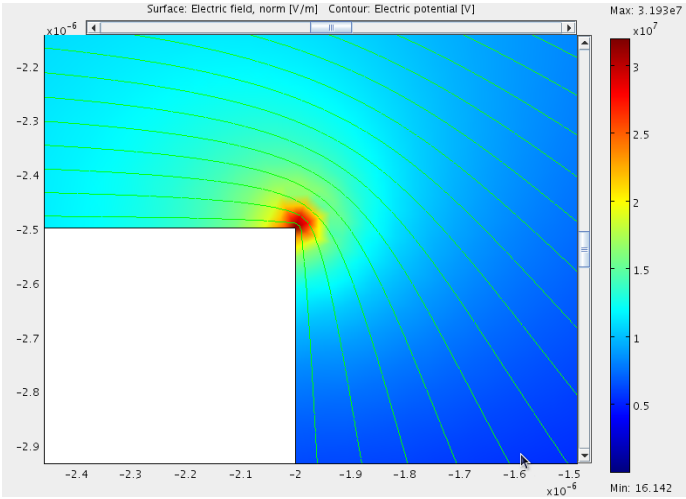




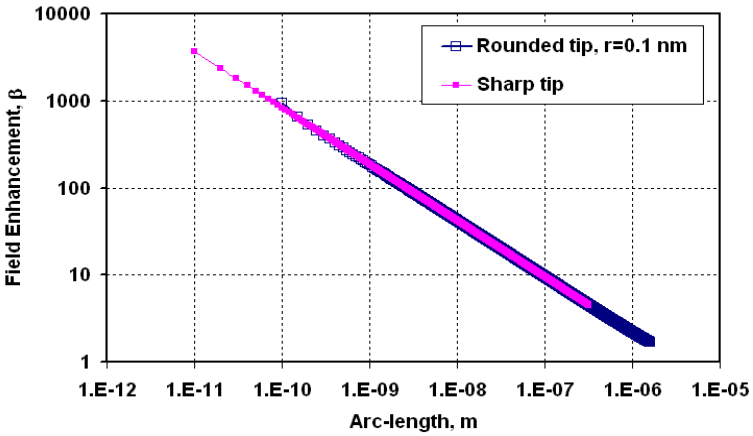


Enhancement at crack's edges

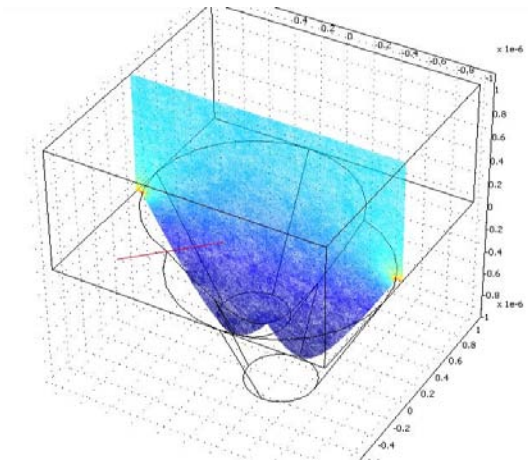
- **Sharp tips, edges and corners of the cracks can significantly enhance the electric field**

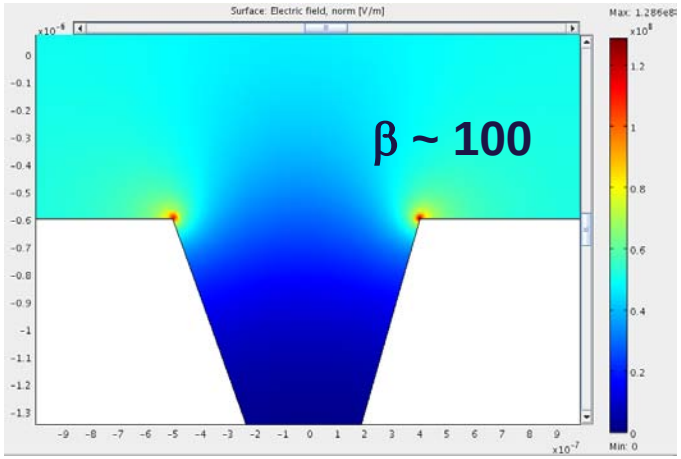


Comparison of FE for two cones: a sharp vs rounded cone



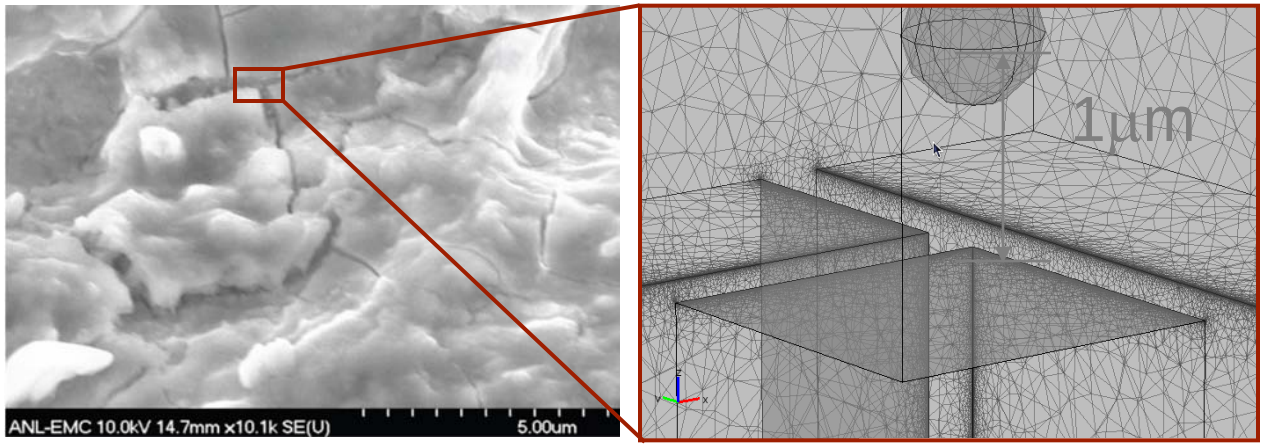
- **More exotic cracks can enhance the electric field too**

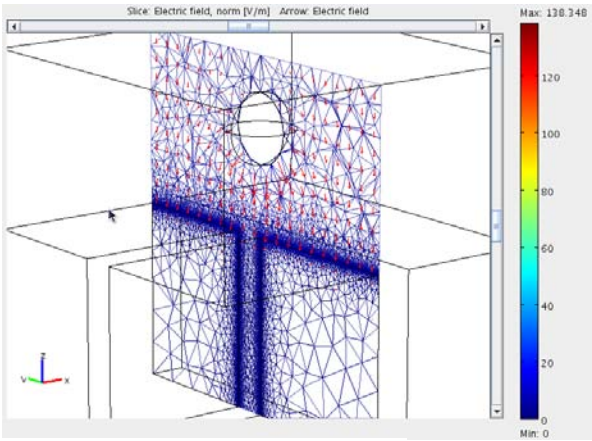


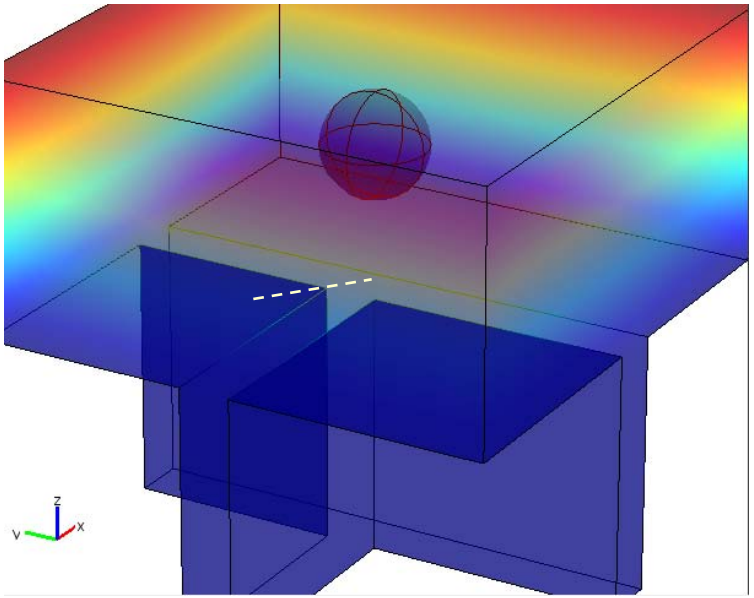


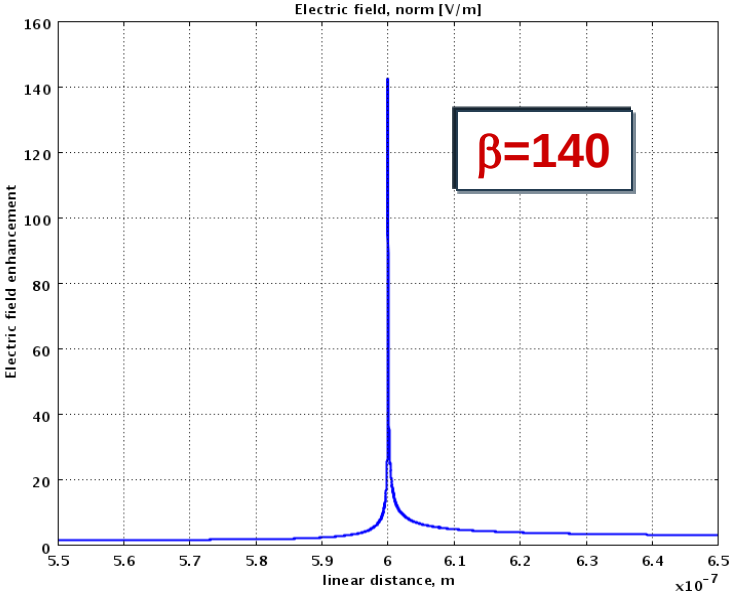
Triple junction E-fields

- **We have been modeling, cracks, junctions, edges and other shapes**
  - **Comsol simulation of field enhancement at triple crack junction**





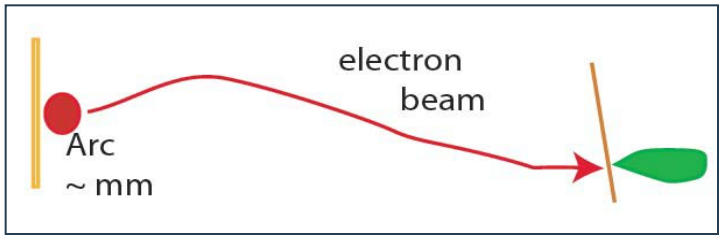




Experimental enhancement factor obtained from dark current measurements: β = 184

Comparison with experiment

X rays show that cavities break down at E_{local} ~ 7–10 GV/m



Fowler-Nordheim field emission (1928)

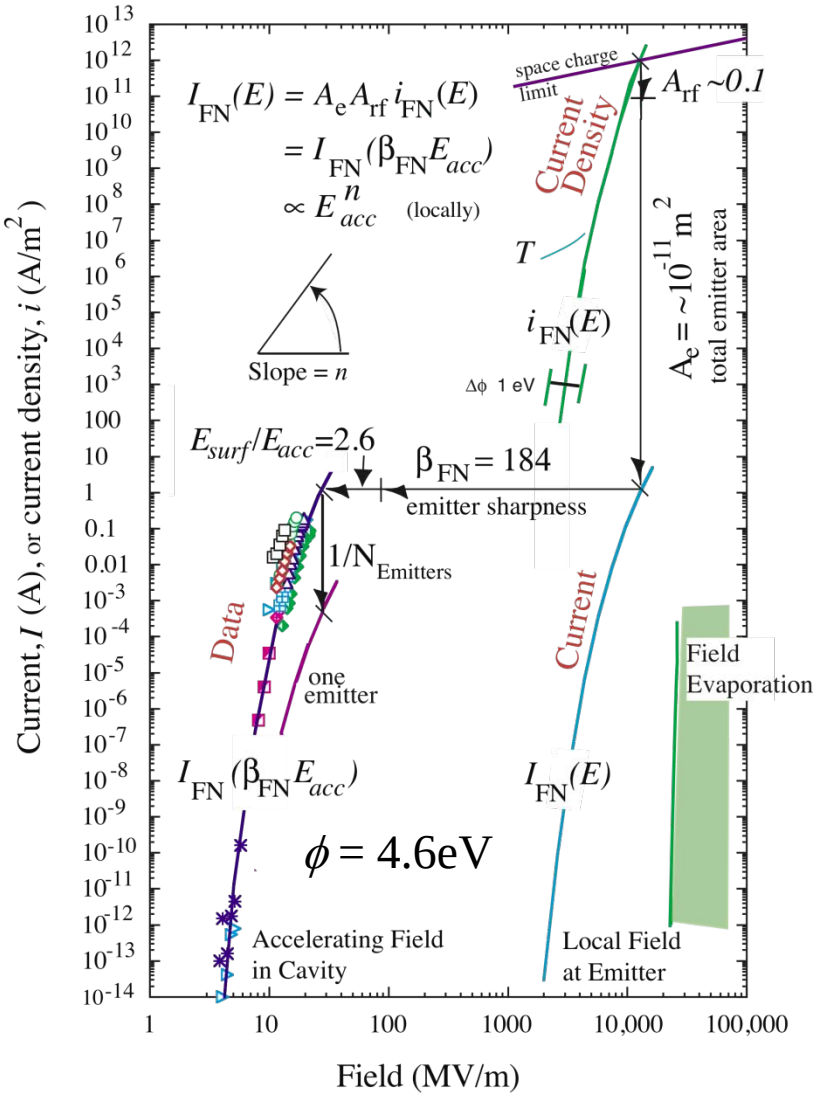
$$i(E_{surf}) = \frac{A_{FN}(\beta E_{surf})^2}{\phi} \exp\left(-\frac{B_{FN}\phi^{3/2}}{\beta E_{surf}}\right), \left(\mathrm{A}/\mathrm{m}^2\right)$$

$$A_{FN} = 1.54\times10^6 \,\mathrm{eV\,A/(MV)^2}$$

$$B_{FN} = 6830\,\mathrm{MV/m(eV)^{3/2}}$$

β – Local Field Enhancement

β=184

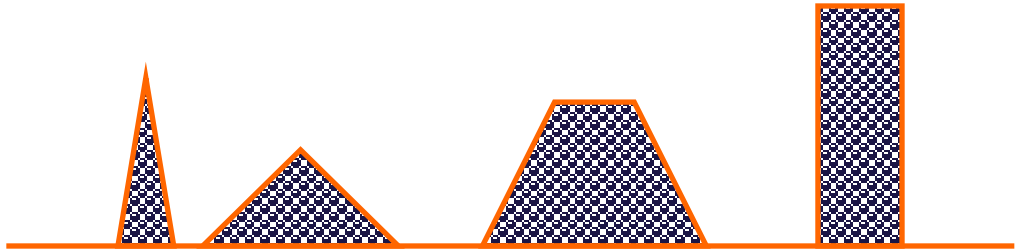


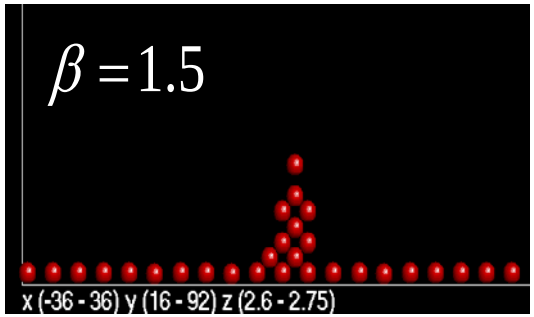
[Norem, PR STAB (2003)]

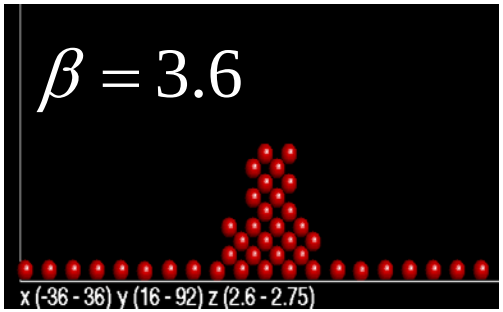
Cluster field evaporation – a result of a high local electric field

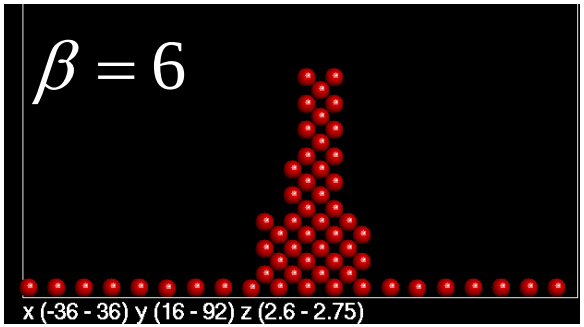
Why atomistic simulation?

Flyura Djurabekova and Kai Nordlund, University of Helsinki

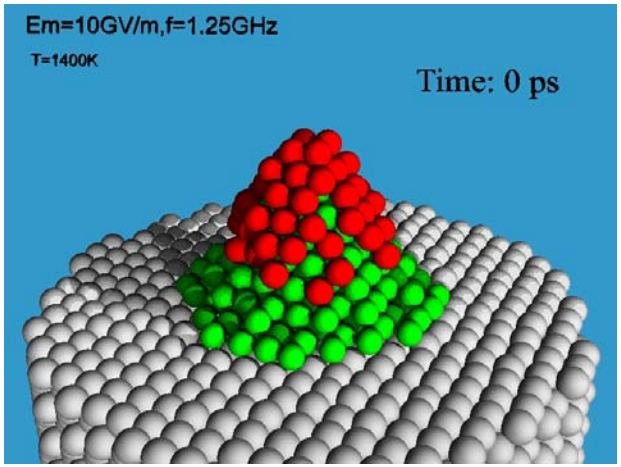


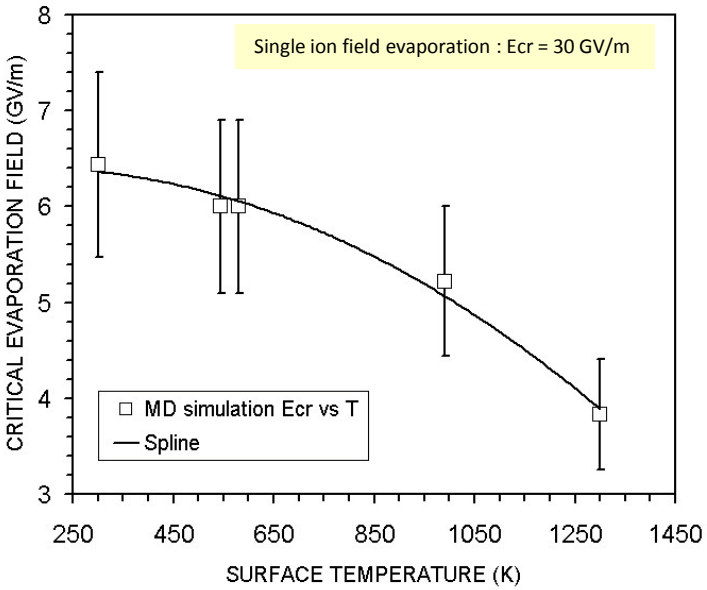






Cluster field evaporation





[Insepov Norem, Phys Rev STAB (2004)]

[Miller, Atom Probe Tomography (2000)]

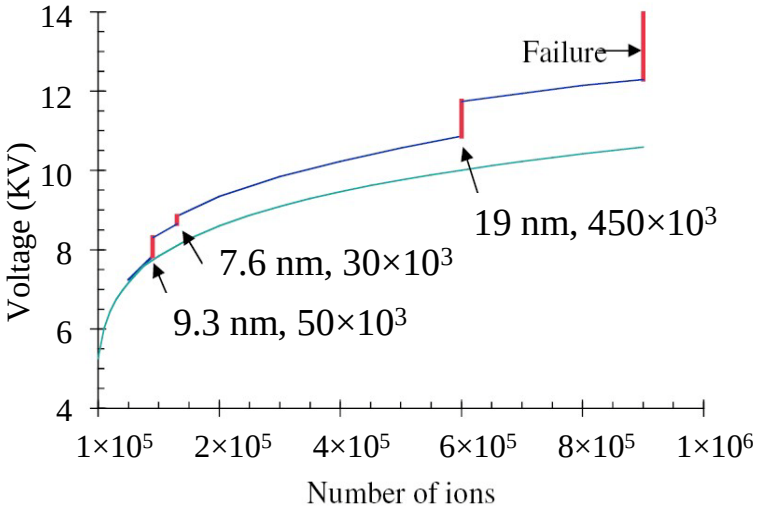
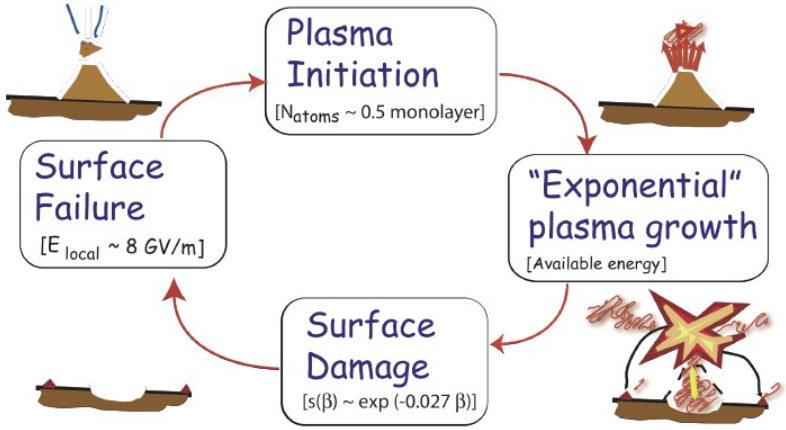
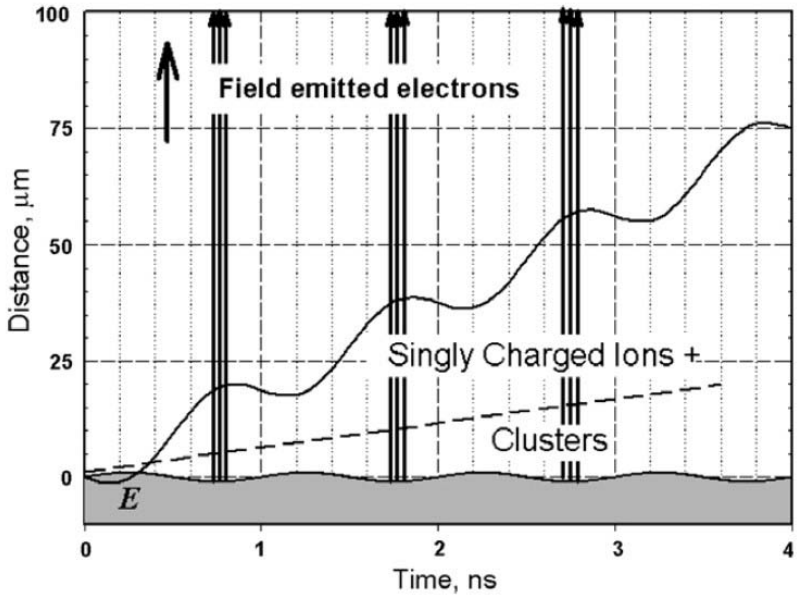


Figure shows abrupt discontinuities in the voltage vs. number of ions in a DC-field evaporation system and evidence for large clusters produced at field ion microscope tips.

Electric field initiates breakdown

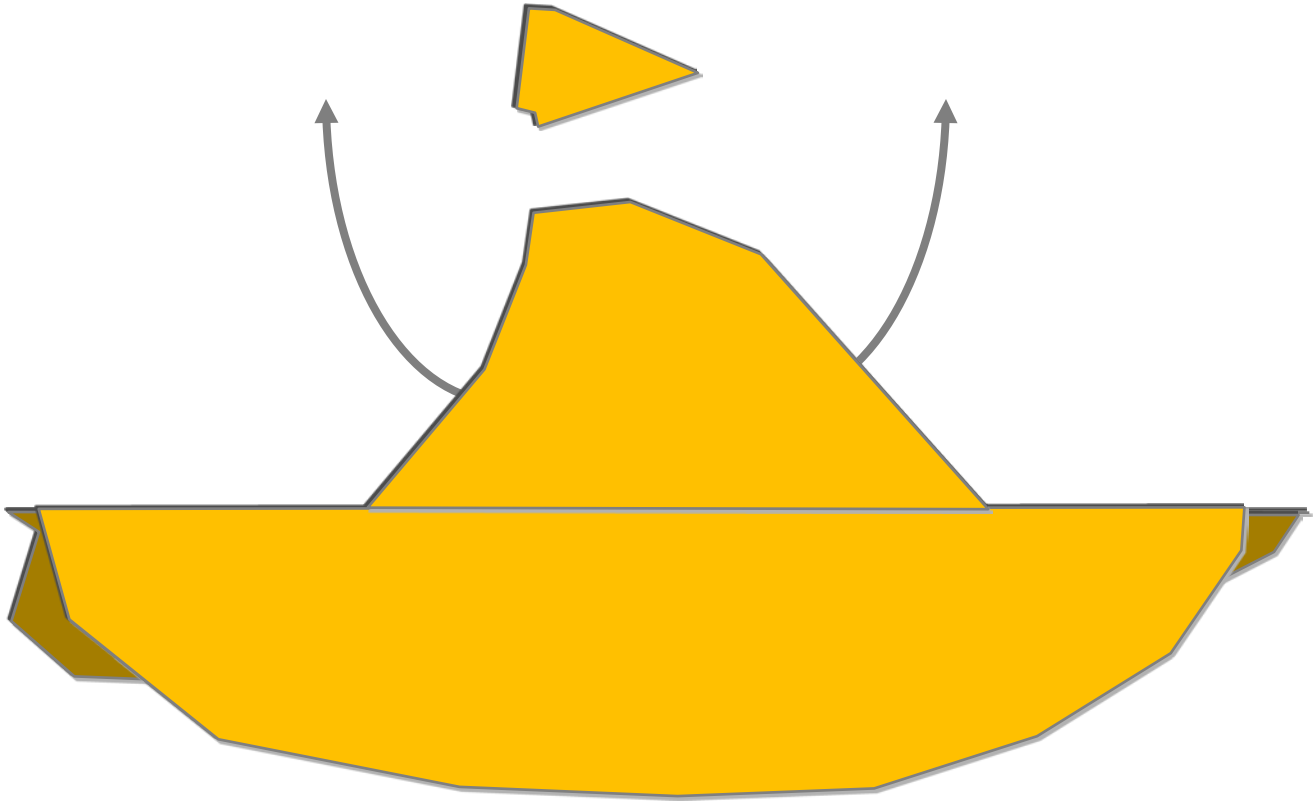
- Surfaces contain grain boundaries, tips, oxides, dust particles
- A strong electrostatic field enhancement can be generated
- Maxwell stress includes electric forces acting on the tip
- The chunks fill the near region of the vacuum
- Ionization by FN-electrons and Coulomb explosion form plasma
- Unipolar plasma model can explain triggering of the breakdown





Crater formation via field evaporation

- **A new mechanism of crater formation – pulling out a large area of the surface**

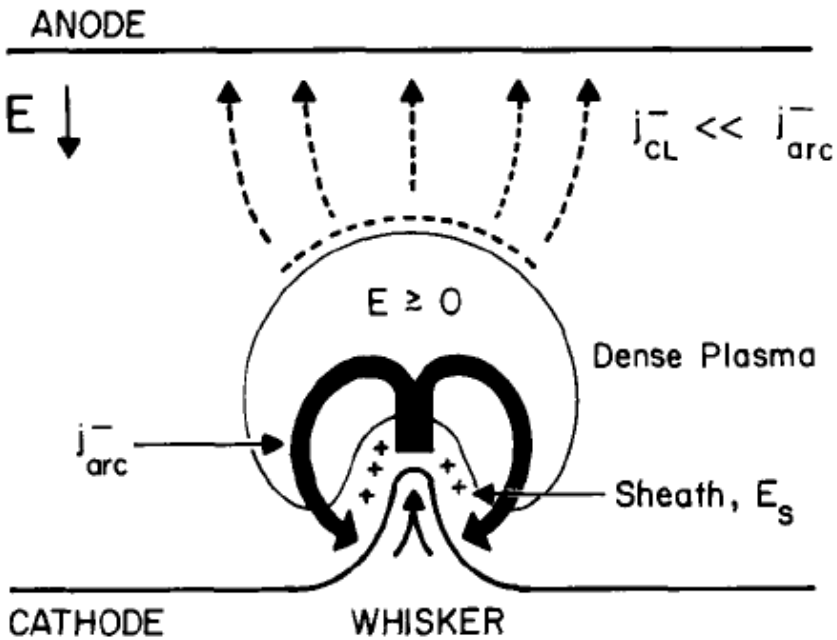


S. Yip, MIT 2014 (private communication)

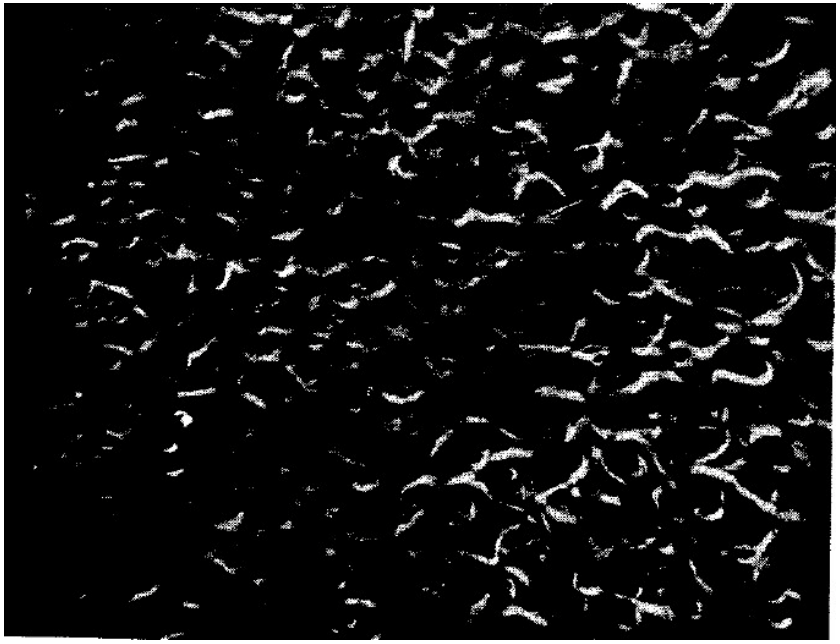
Unipolar (Schwirzke) Plasma model development

Double electric layer in plasma

Tokamak

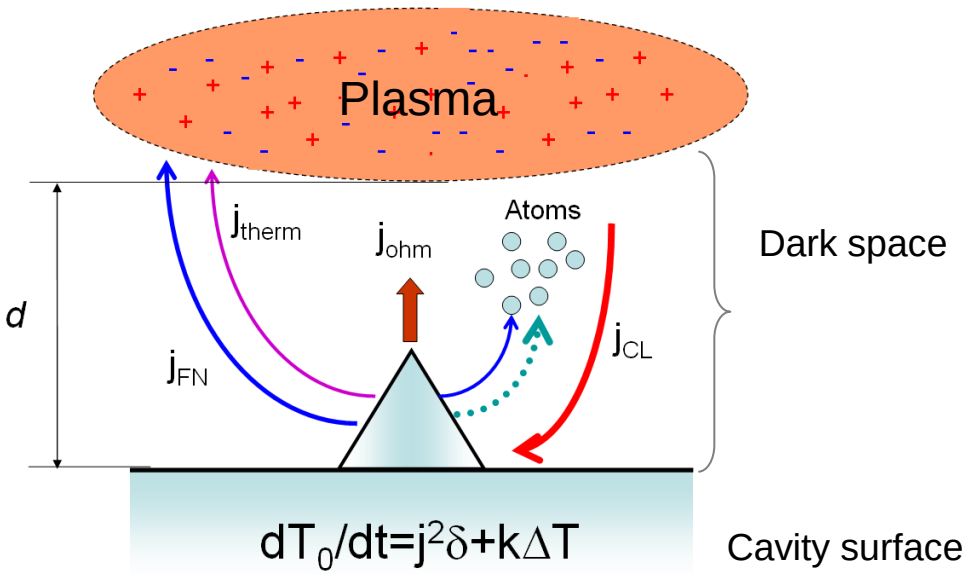


F. R. Schwirzke,
IEEE Trans. on Plas. Sci., **19**, 690 (1991)



SEM image of plasma damaged metal surface: Superposition of “younger” (10 μm) and “older” craters (30-40 μm).

Unipolar arc breakdown model



BD triggered by impact ionization

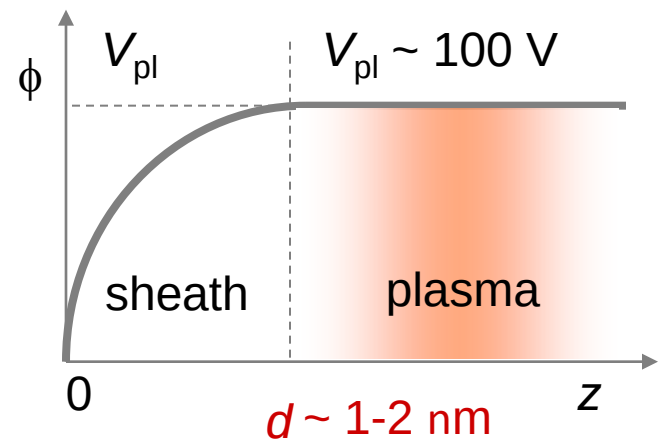
- **Neutrals accumulated in the dark space**
- **Ionization of neutrals by FN-current**
- **Percolation of dark space via ionization**
- **Crater formation via explosion**

Unipolar Arc Model

$$V_{pl} = \frac{k_B T_e}{2e} \ln\left(\frac{M_i}{2\pi m_e}\right),$$ Plasma potential

$$E_s = V_{pl} / \lambda_d,$$ Surface field

$$\lambda_d = \left(\frac{\varepsilon_0 V_{pl}}{n_e e^2}\right)^{1/2}$$ Debye length



Unipolar Arc model in linac

Heating occurs via ion bombardment.
Plasma fueling:

- Evaporation of surface atoms
- Tip explosion by high electric field

Plasma potential

$$U_f = \left(\frac{kT_e}{2e}\right)\ln\left(\frac{M_i}{2\pi m_e}\right),$$

$$\lambda_D = \sqrt{\frac{\varepsilon_0 kT_e}{2n_e e^2}},$$

$$E_f \approx \frac{U_f}{\lambda_D} \approx (n_e kT_e)^{1/2} \times 5.12$$

$$n_e \approx 1\times10^{25}\ m^{-3}$$

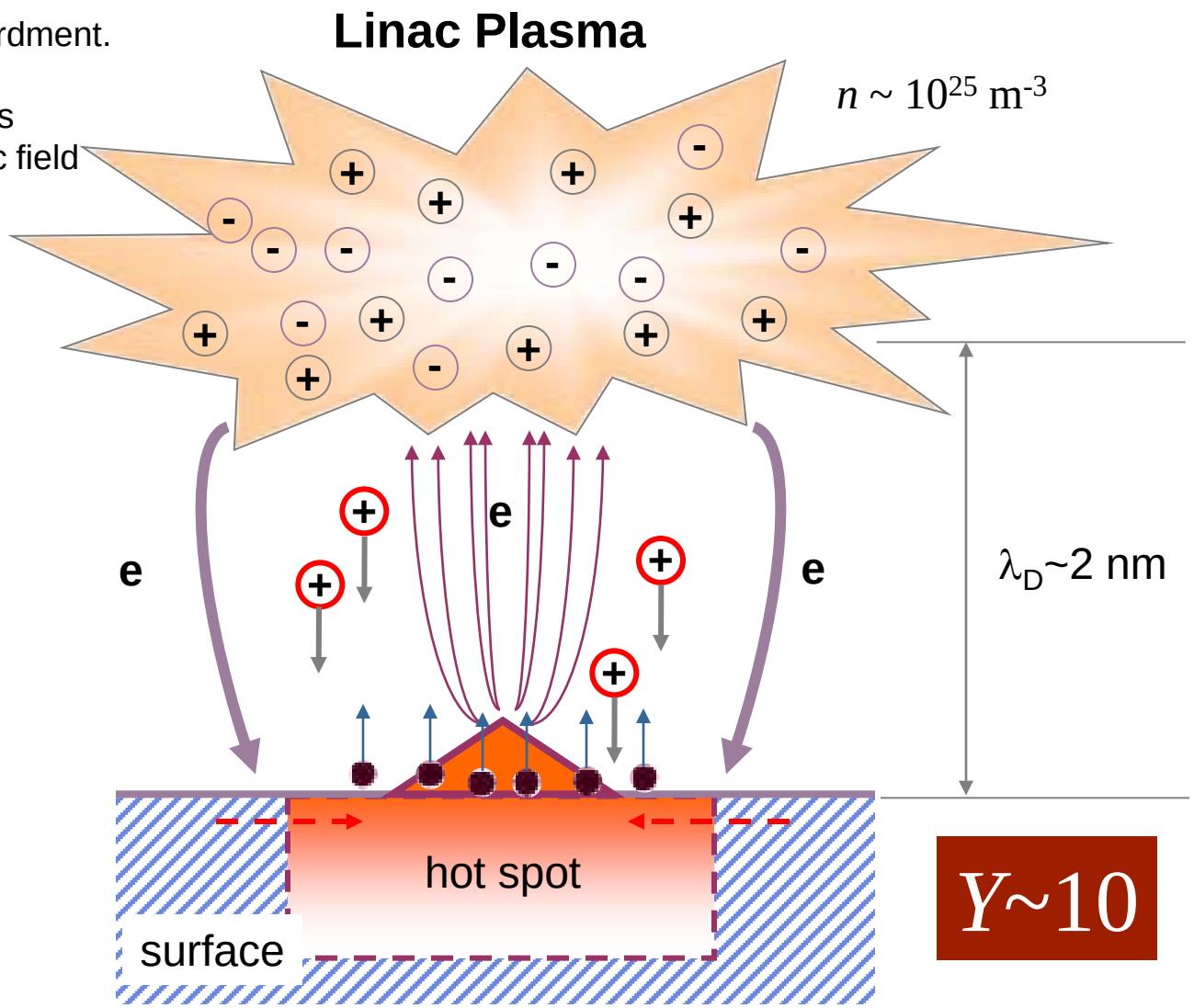
$$kT_e \approx 18\,eV, U_f \approx 50\,V$$

$$\lambda_D \approx 2\times10^{-9}\,m,$$

$$d_c \approx 1.5\times\lambda_D$$

$$E_f \approx \beta\frac{U_f}{\lambda_D} \approx 5\times10^{10}\,V/m$$

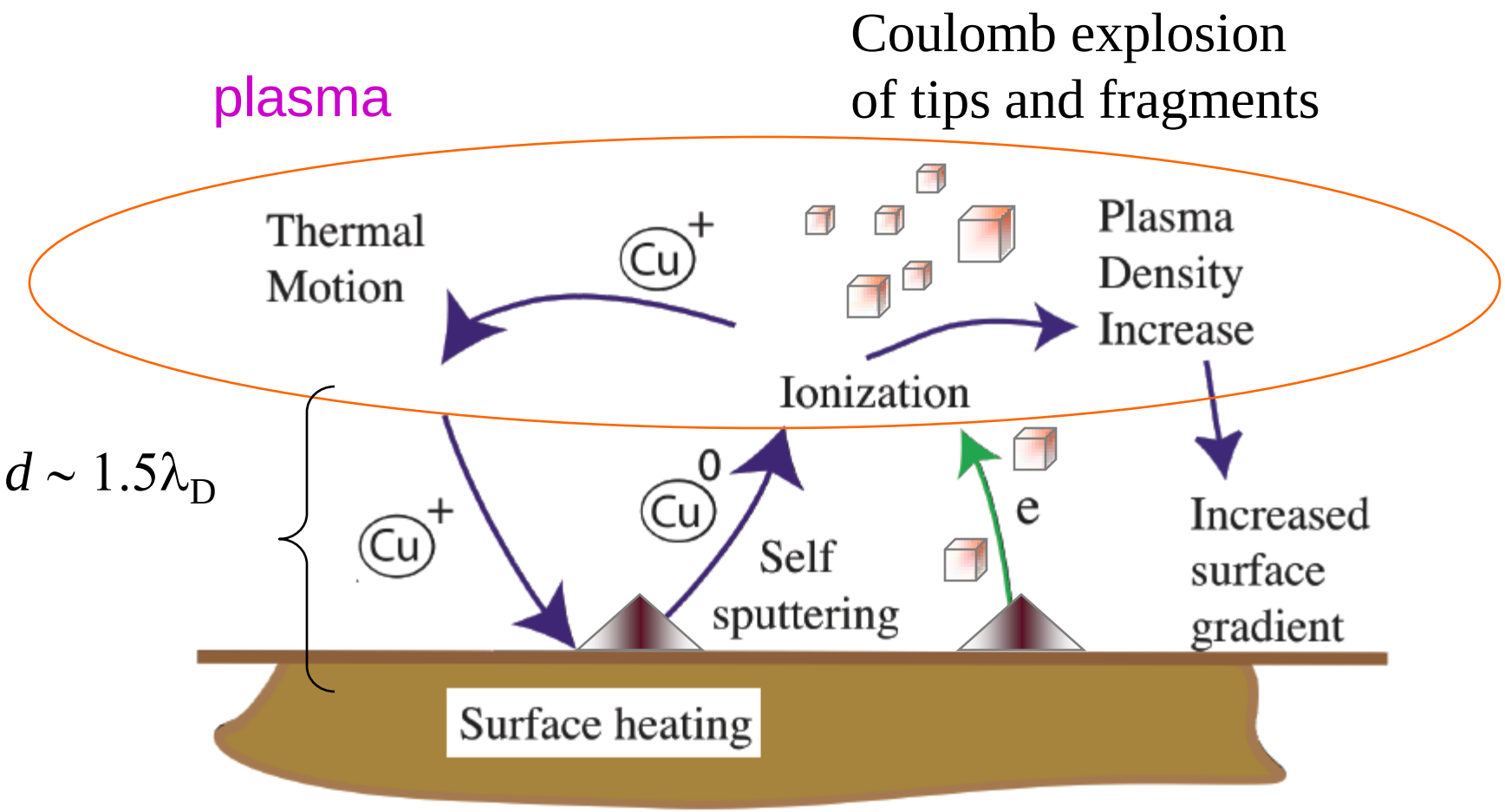
[Insepov, Norem, 2012]



Y~10

- Schwirzke model

Self-sputtering by plasma



Self-sputtering is the main mechanism of plasma fueling

Surface sputtering by ions

- **Sigmund's theory** – linear cascades, not good for heavy ions and low energies
- **Monte Carlo codes**: binary collisions, not accurate at low energies
- **Empirical models** based on MC – good for known materials
- **Molecular dynamics** – time consuming but no limit for energies, ion masses, temperatures, dense cascades, thermal properties - can verify the OOPIC/VORPAL simulations

Sputtering theory and models

- **Sigmund's theory**

$$Y(E) = \Lambda F_D(E),$$

$$\Lambda = \frac{3}{4\pi^2}\frac{1}{NC_0U_s} = \frac{0.0420}{NU_s},$$

$$F_D(E) = \alpha(M_2/M_1)NS_n(E)$$

$F_D(E)$ – deposited energy,

N – atomic density,

U_s - surface binding energy,

$S_n(E)$ – nuclear stopping power,

C_0 – coefficient.

Not applicable for heavy ions
C_0, U_s - adjustable parameter.

[P. Sigmund, Phys. Rev. B (1969)]

- **Eckstein-Bohdansky's model**

$$Y(E) = Qs_n(\varepsilon)\left[1-\left(\frac{E_{th}}{E}\right)^{2/3}\right]\left[1-\left(\frac{E_{th}}{E}\right)\right]^2,$$

Q, E_{th} – adjustable parameters,

$$\varepsilon = E\frac{M_2}{M_1+M_2}\frac{a_L}{Z_1Z_2e^2}, (\varepsilon \text{ - reduced energy})$$

$$a_L = 0.4685\left\{Z_1^{2/3}+Z_2^{2/3}\right\}^{-1/2}\text{A}$$

$$s_n^{TF}(\varepsilon) = \frac{3.441\sqrt{\varepsilon}\ln(1+1.2288\varepsilon)}{\varepsilon+0.1728\sqrt{\varepsilon}+\varepsilon\left(6.882\sqrt{\varepsilon}-1.708\right)}.$$

Not applicable for light ion, high energy ions
(no electronic stopping power).
Needs adjustable parameters.

[Bohdansky, NIMB B (1984)]

Yamamura's empirical model

- **Yamamura's interpolation model based on Monte-Carlo code**

$$Y(E) = 0.042\frac{F_D(E)}{NU_s}\left[1-\sqrt{\frac{E_{th}}{E}}\right] =$$

$$0.042\frac{\alpha(M_2/M_1)S_n(E)}{NU_s}\left[1-\sqrt{\frac{E_{th}}{E}}\right]$$

N – atomic density, U_s - surface binding energy,

$S_n(E)$ – nuclear stopping power,

α – adjustable parameter,

$$Y(E) = 0.042\frac{\alpha(M_2/M_1)}{U_s}\frac{S_n(E)s_n(\varepsilon)}{s_n(\varepsilon)+S_n(E)}\times\left[1-\sqrt{\frac{E_{th}}{E}}\right]^s,$$

$$E_{th} = \begin{cases} \dfrac{6.7}{\gamma}, & M_1 \geq M_2, \\ \dfrac{1+5.7(M_1/M_2)}{\gamma}, & M_1 \leq M_2. \end{cases}$$

$$\gamma = \frac{4M_1M_2}{(M_1+M_2)^2}.$$

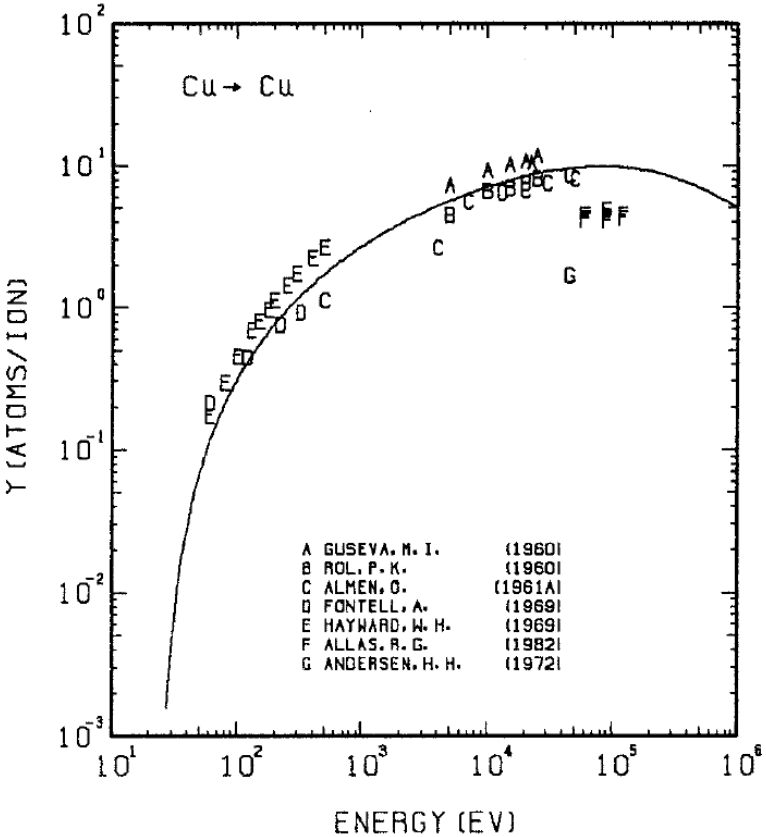
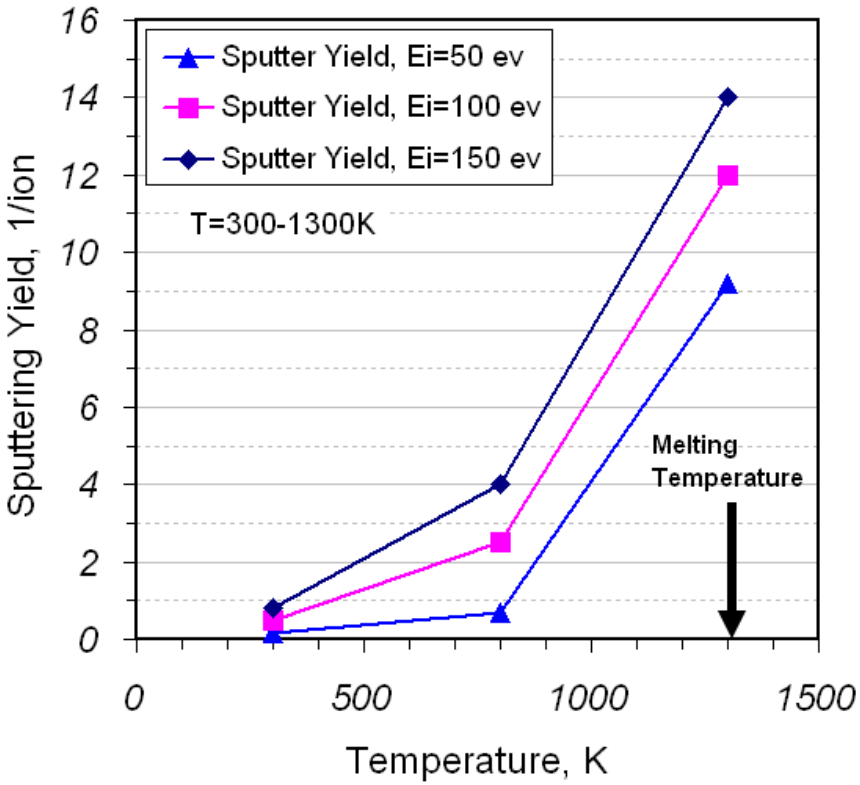
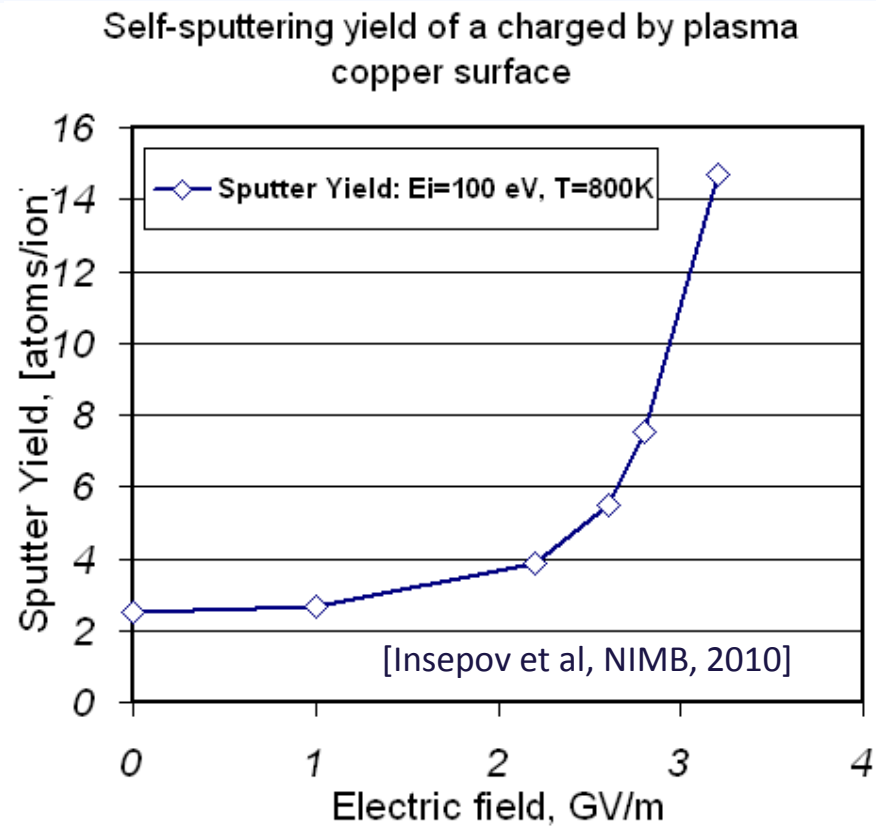


FIG. 123 ENERGY DEPENDENCE OF THE SPUTTERING YIELD OF CU WITH CU^+.
A= 1.00, Q= 1.00, Us= 3.49EV, s= 2.50, W= 0.21Us.

No temperature dependence

MD simulation of Copper self-sputtering at high T and E

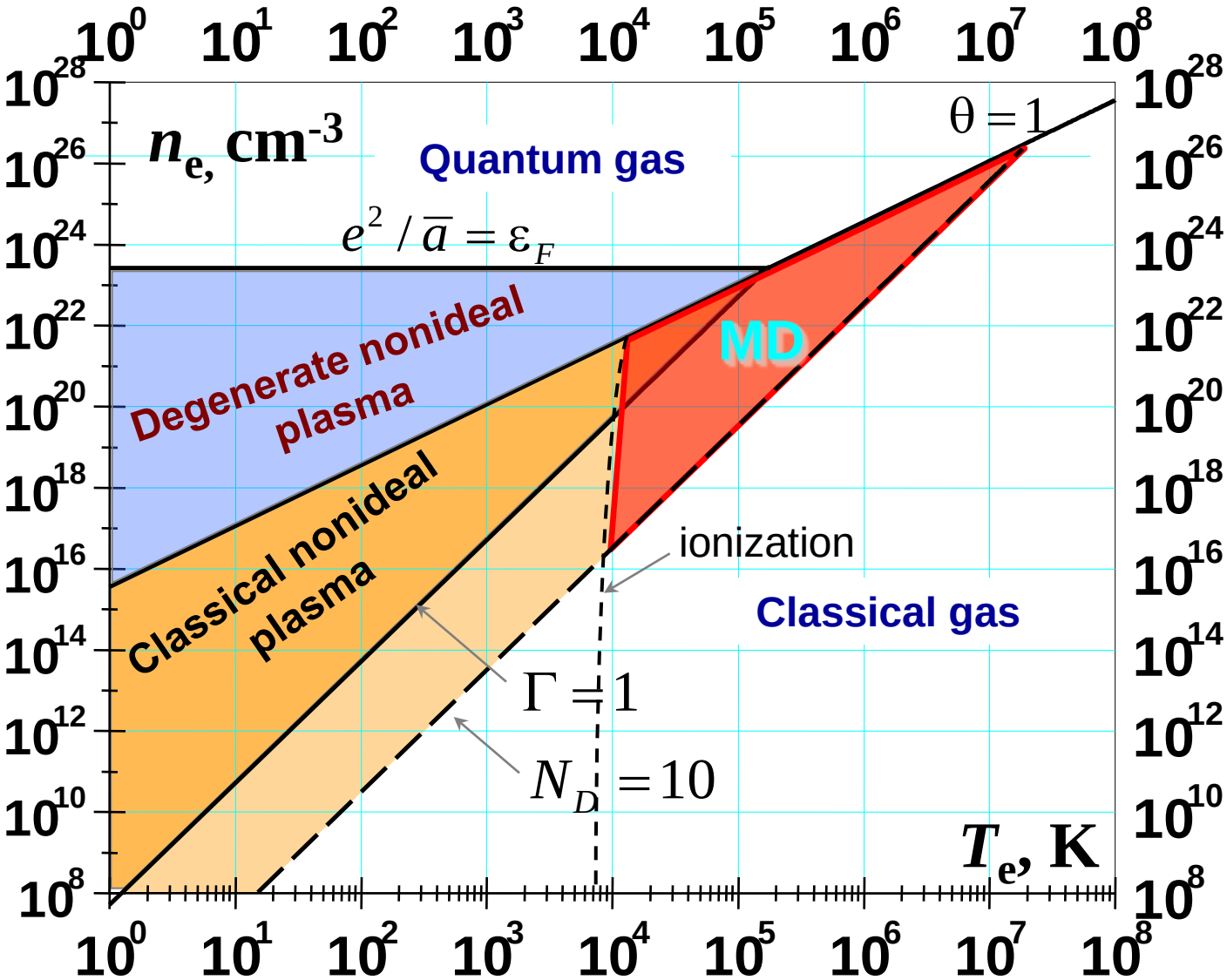




- **Self-sputtering is the mechanism for fueling unipolar surface plasma.**
- **Unipolar model requires Y > 10 typical at low ion energies.**
- **MD predicts very high sputtering yields for high surface *T* and *E*.**
- **Erosion rates on the order of ~ 1 m/s.**

Atomistic model of non-Debye near-surface plasma

n-T Diagram for plasmas



Nonideality parameter for electrons

$$\Gamma = \left(\frac{4\pi n_e}{3}\right)^{1/3} \frac{e^2}{kT}$$

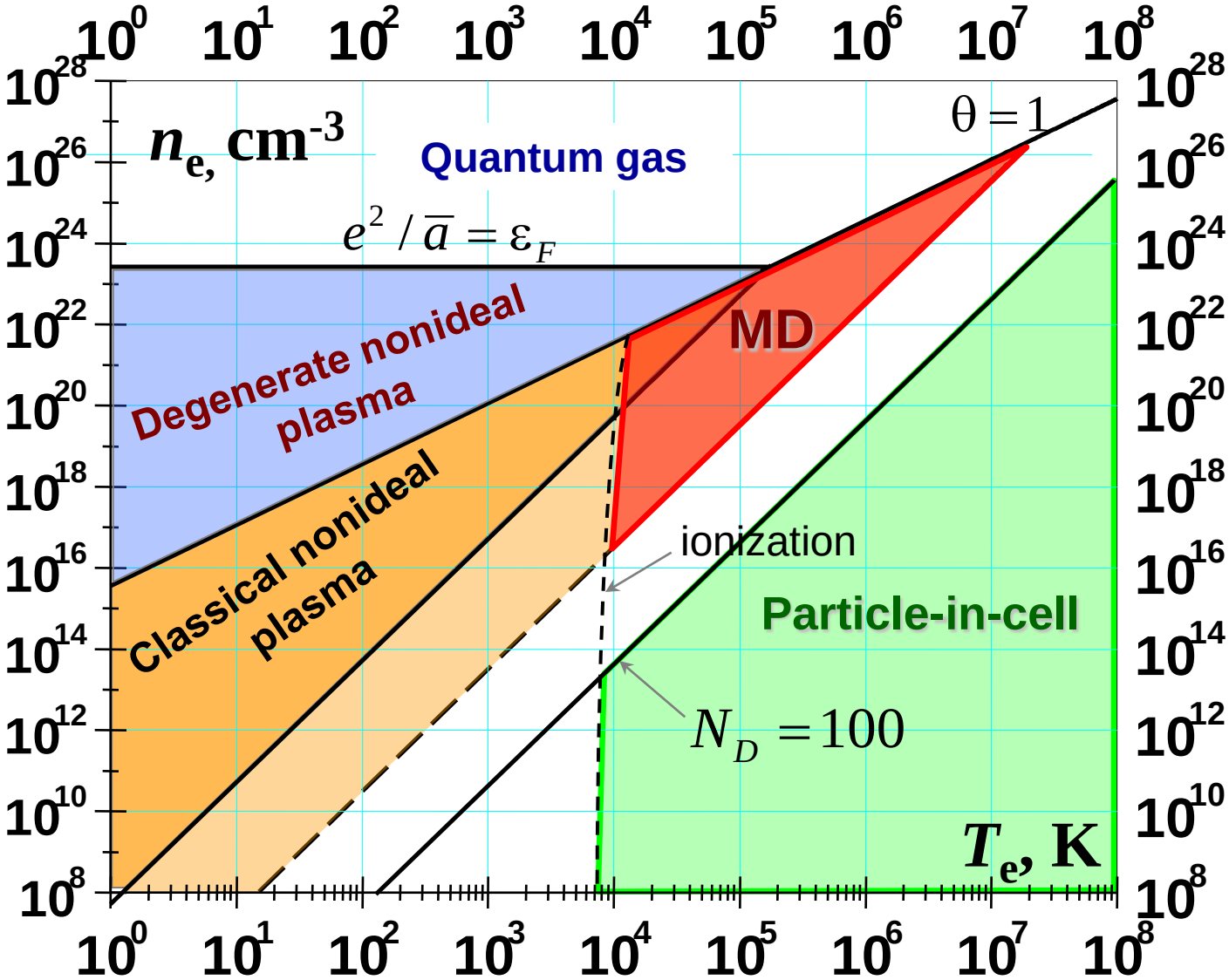
Number of electrons in the Debye sphere

$$N_D = \frac{4\pi r_D^3}{3} n_e$$

Degeneracy parameter

$$\theta = \varepsilon_F / kT$$

Density-Temperature Diagram



Nonideality parameter for electrons

$$\Gamma = \left(\frac{4\pi n_e}{3}\right)^{1/3} \frac{e^2}{kT}$$

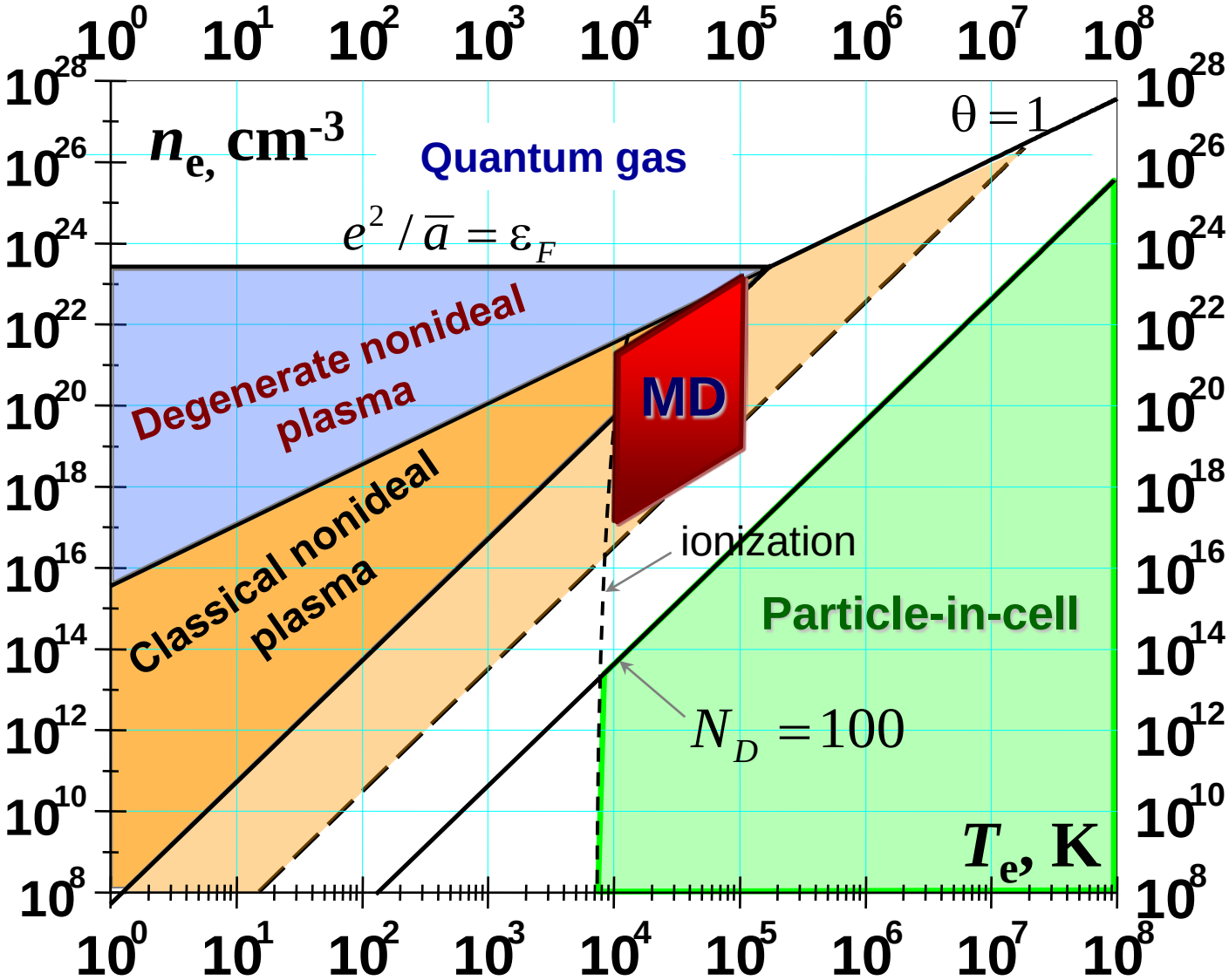
Number of electrons in the Debye sphere

$$N_D = \frac{4\pi r_D^3}{3} n_e$$

Degeneracy parameter

$$\theta = \varepsilon_F / kT$$

Density-Temperature Diagram



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Number of electrons in the Debye sphere

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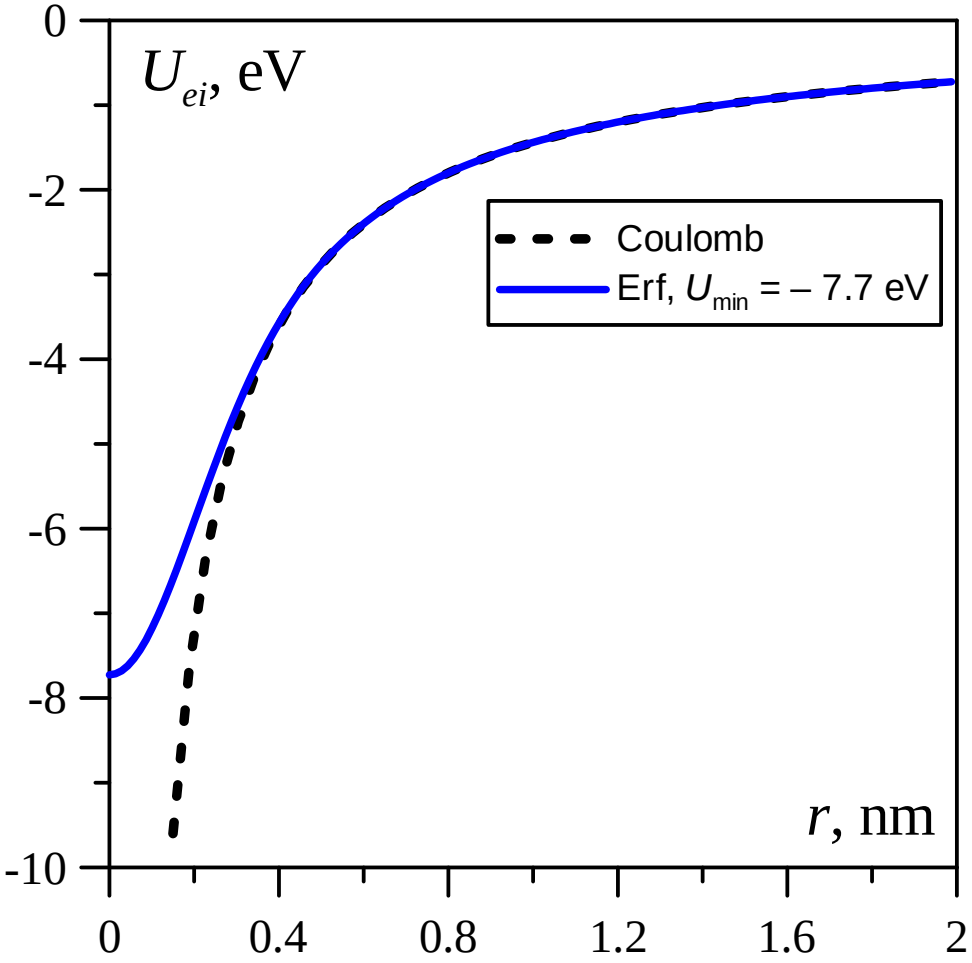
Degeneracy parameter

$$\theta = \varepsilon_F / kT$$

Simulation Features

- Classical molecular dynamics (MD) simulations with a pseudopotential to account for quantum effects
- Two component plasma of electrons and copper ions
- Long range Coulomb interactions (*N*-body problem)
- Nearest image method (periodical boundary conditions) for the transversal dimensions
- Absorption of electrons to the surface with generation of the surface electrostatic field
- Simulation of the relaxation process
- Averaging over an ensemble of initial states

Interaction Potentials



Electron-ion interaction potential

$$U_{ei}(r) = -\frac{Ze^2}{r}\,\mathrm{erf}\left(\frac{r}{\sigma}\right)$$

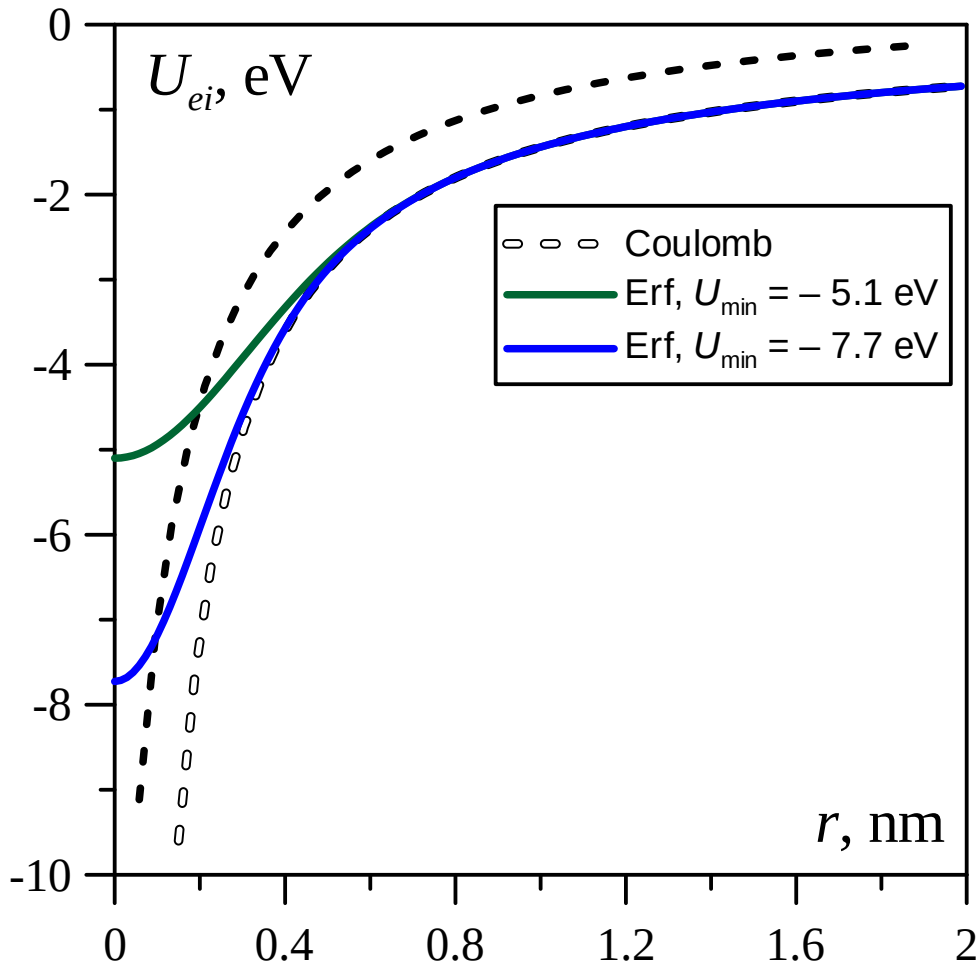
Ionization potential for Copper

$\boldsymbol{U_{min} = U_{ei}(0) = -7.73}$ **eV**

(σ = 0.21nm)

Electron-electron and ion-ion potentials are pure Coulomb. The erf-like electron-ion interaction potential given above was used e.g. for simulations of sodium clusters in *T. Raitza, H. Reinholz, G. Röpke, I. Morozov, E. Suraud, Contrib. Plasma Phys* ***49*** *496 (2009).*

Interaction Potentials



Electron-ion interaction potential

$$U_{ei}(r) = -\frac{Ze^2}{r}\,\mathrm{erf}\left(\frac{r}{\sigma}\right)$$

Ionization potential for Copper

$$U_{min} = U_{ei}(0) = -7.73 \text{ eV}$$

(σ = 0.21nm)

Test potential

$$U_{min} = U_{ei}(0) = -5.1 \text{ eV}$$

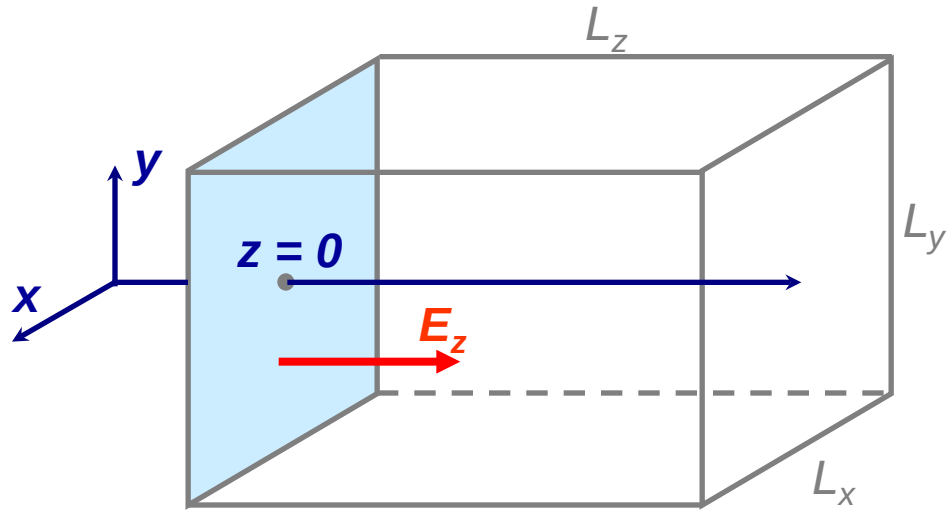
(σ = 0.32nm)

Electron-electron and ion-ion potentials were pure Coulomb. The erf-like electron-ion interaction potential shown above was previously used for simulations of sodium clusters in [T. Raitza et al, Contrib. Plasma Phys (2009)].

Surface electric field in box

$$a = \frac{L_x}{2} = \frac{L_y}{2}$$

$$\sigma = \frac{q}{L_x L_y}$$ (charge density)



Electric potential on z axis

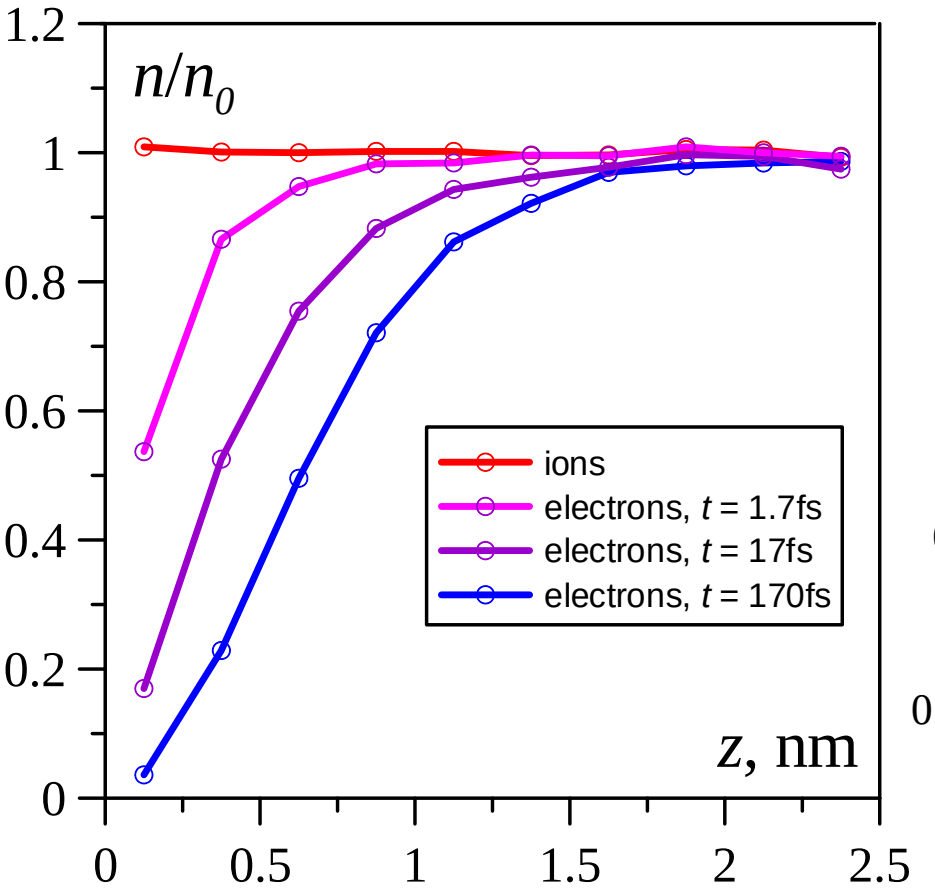
$$\phi(z) = -\frac{\sigma}{4\pi\varepsilon_0} \int_{-L_x/2}^{L_x/2} dx \int_{-L_y/2}^{L_y/2} dy \frac{1}{\sqrt{x^2 + y^2 + z^2}}$$

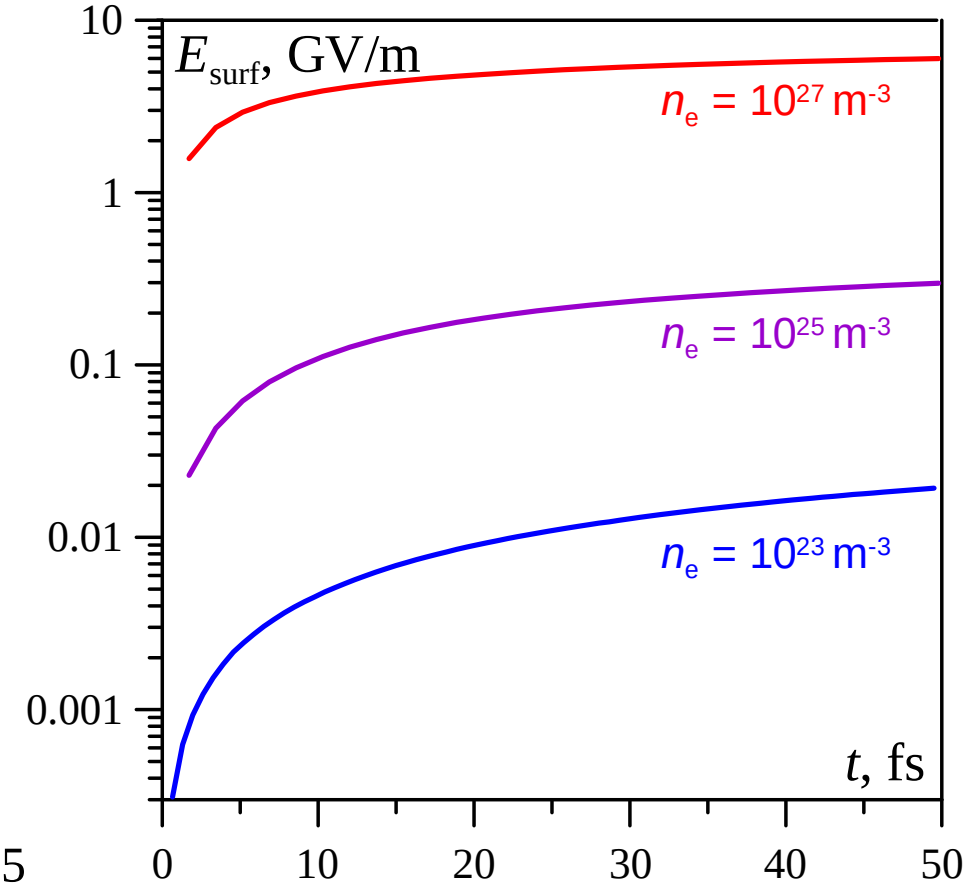
$$= -\frac{\sigma}{\pi\varepsilon_0}\left(z \arctan\left[\frac{a^2}{z\sqrt{2a^2 + z^2}}\right] + a \log\left[\frac{\sqrt{2a^2 + z^2} - a}{\sqrt{2a^2 + z^2} + a}\right]\right)$$

Longitudinal component of the electric field

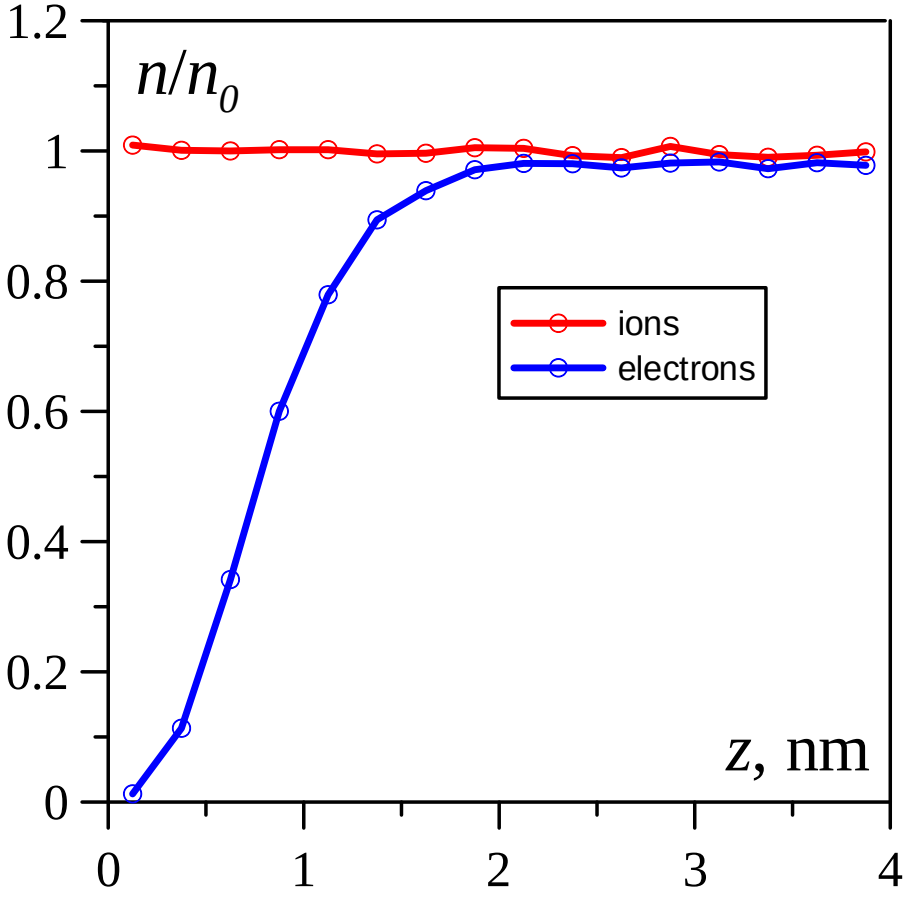
$$E_z(z) = -\frac{\partial \phi}{\partial z} = \frac{\sigma}{\pi\varepsilon_0} \arctan\left[\frac{a^2}{z\sqrt{2a^2 + z^2}}\right]$$

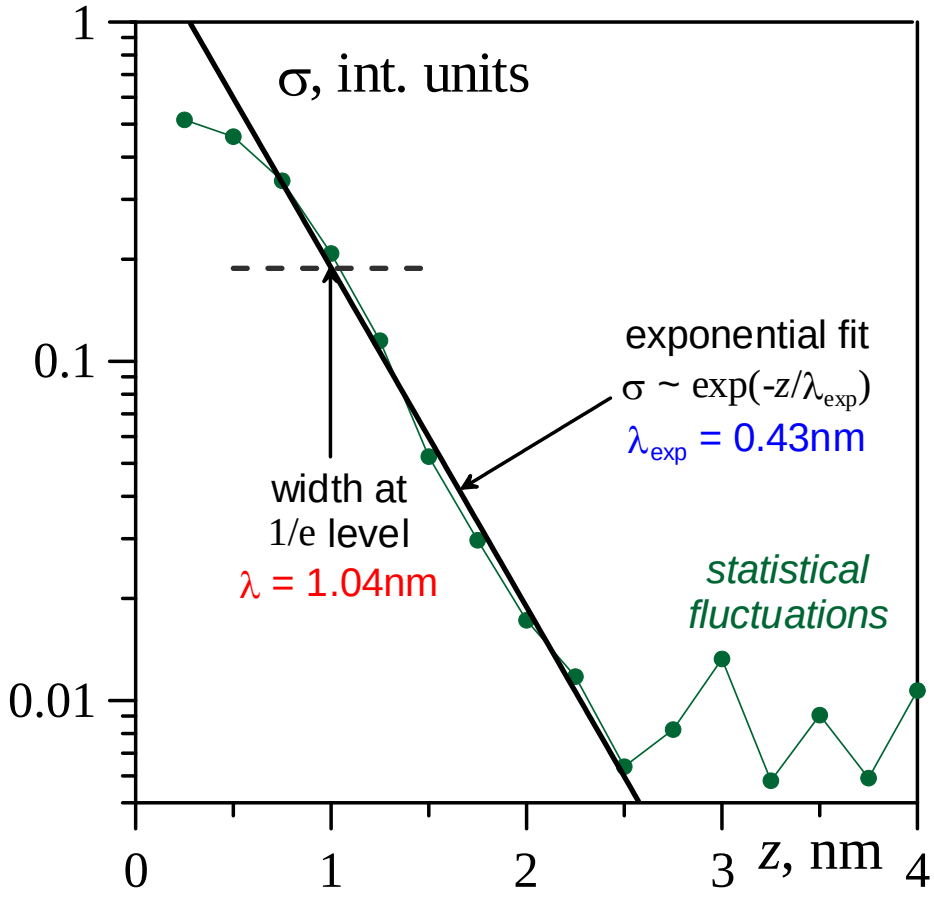
E-field and density vs time





Stationary plasma sheath





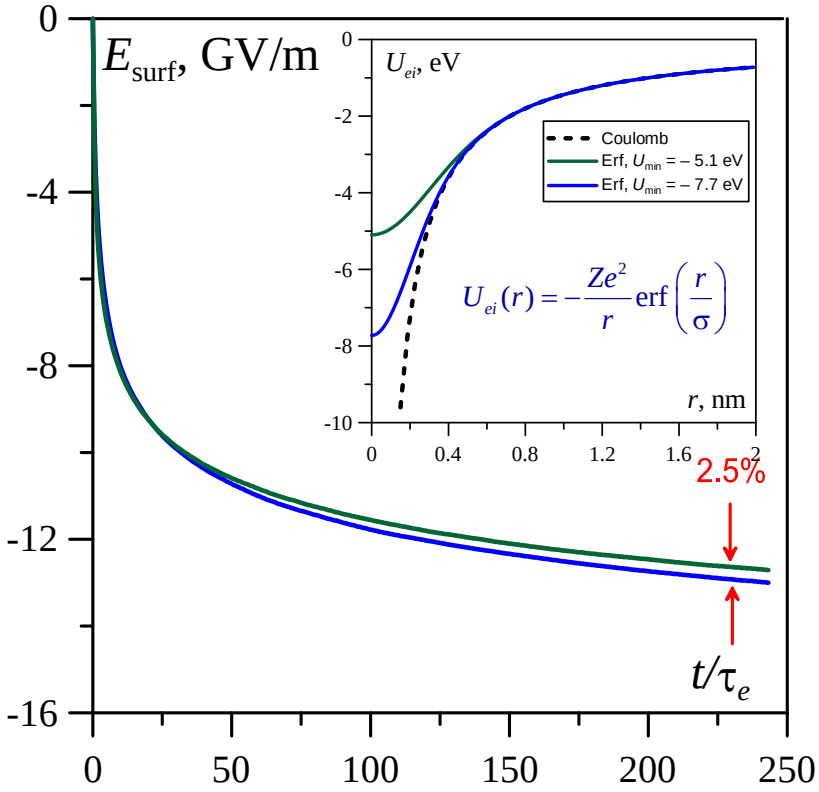
$$T_e = 1\text{eV}, \quad n_0 = 10^{27}\text{m}^{-3}, \quad \Gamma = 2.32$$

Effect of Interaction potential

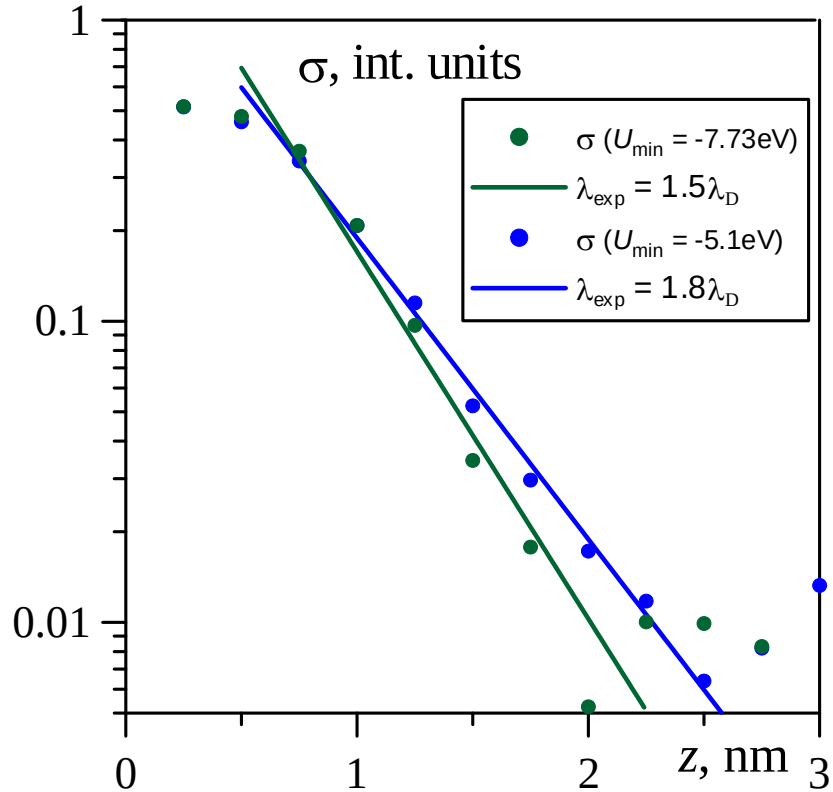
The parameters used in this paper U_{min} **= - 7.73 eV** (σ = 0.21nm)

Test potential: U_{min} = - 5.1 eV (σ = 0.32nm)

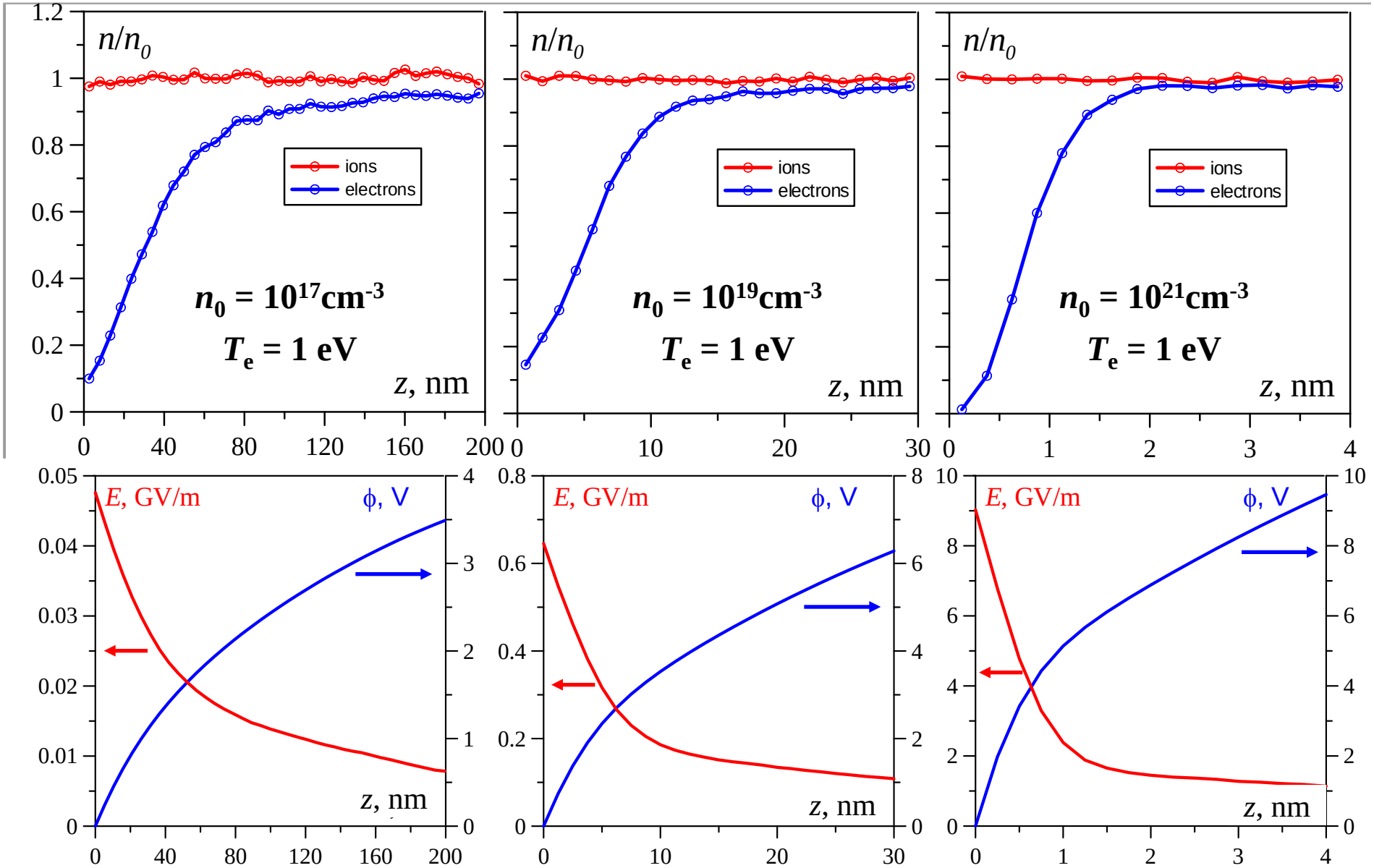
Relaxation of the surface field



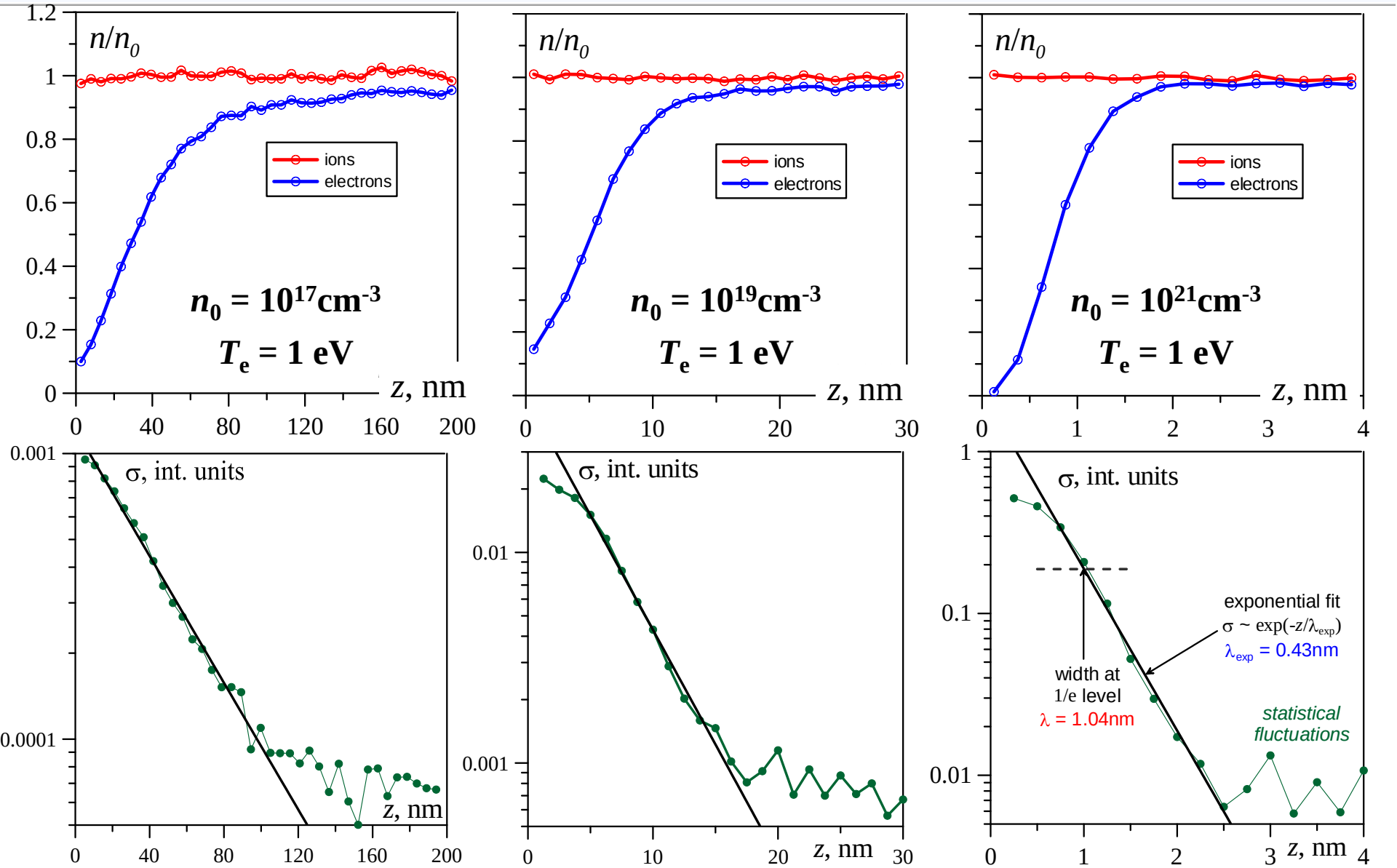
Charge distribution in the sheath area



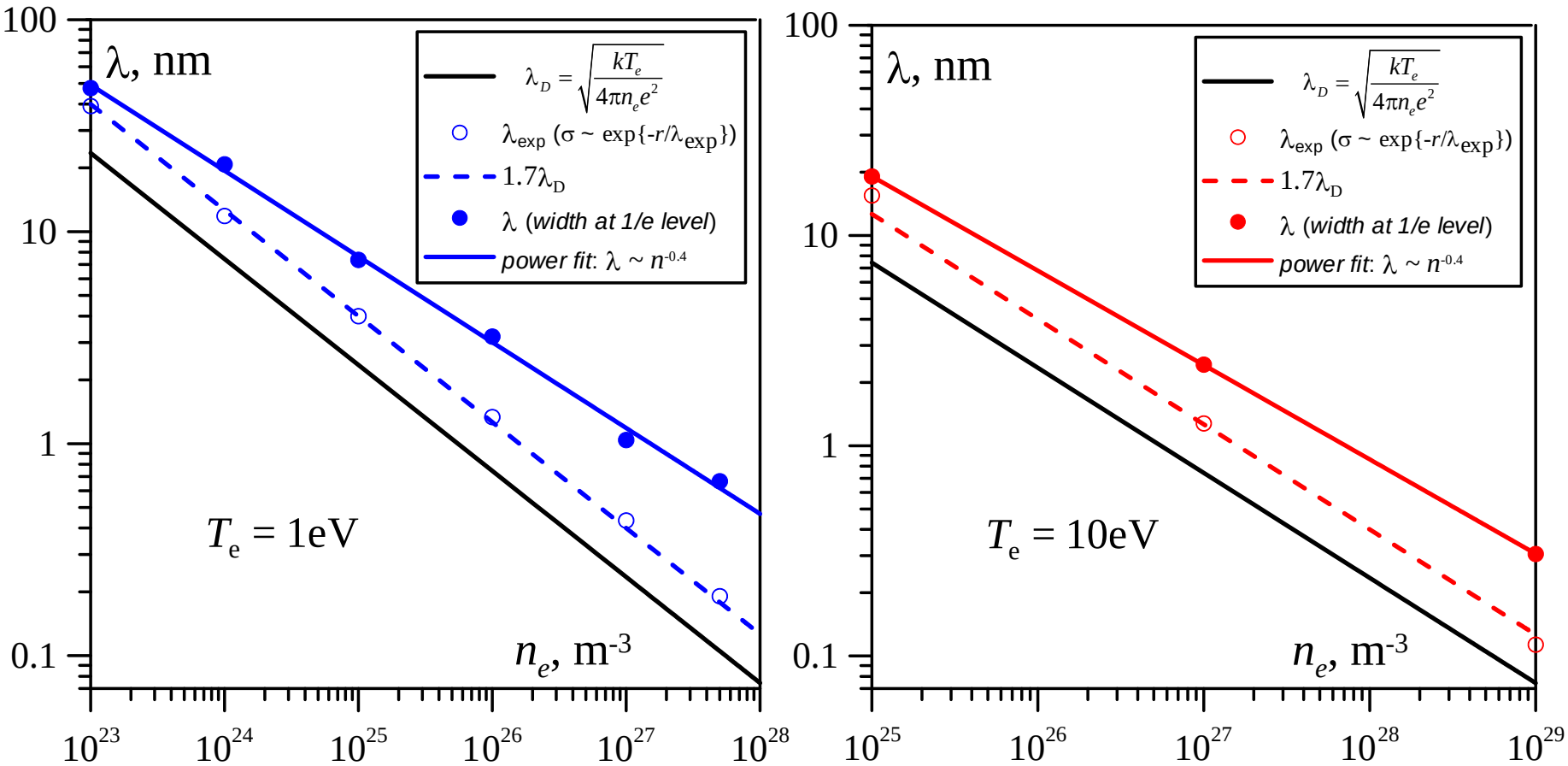
Sheath for stationary state



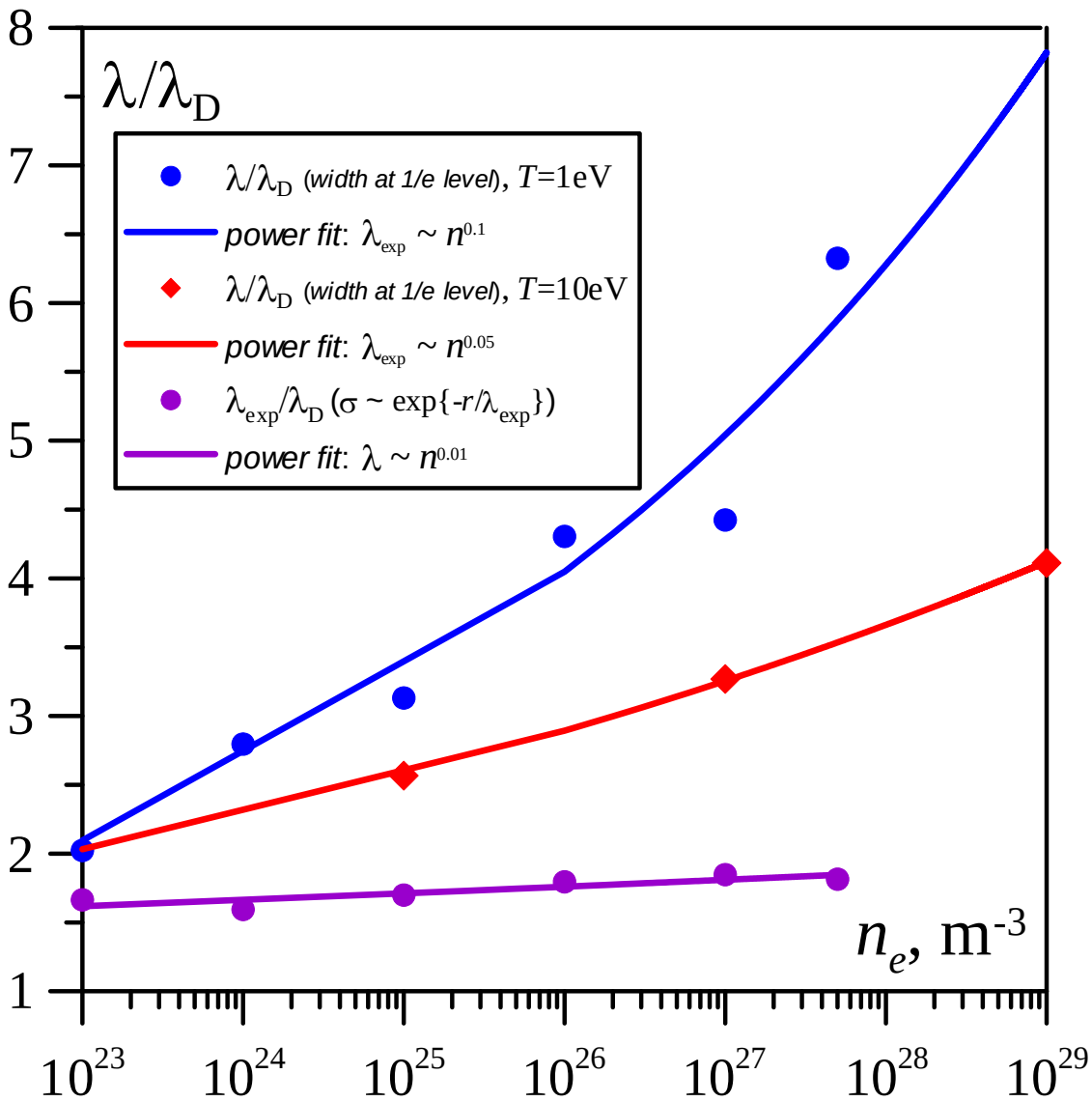
Sheath for stationary state



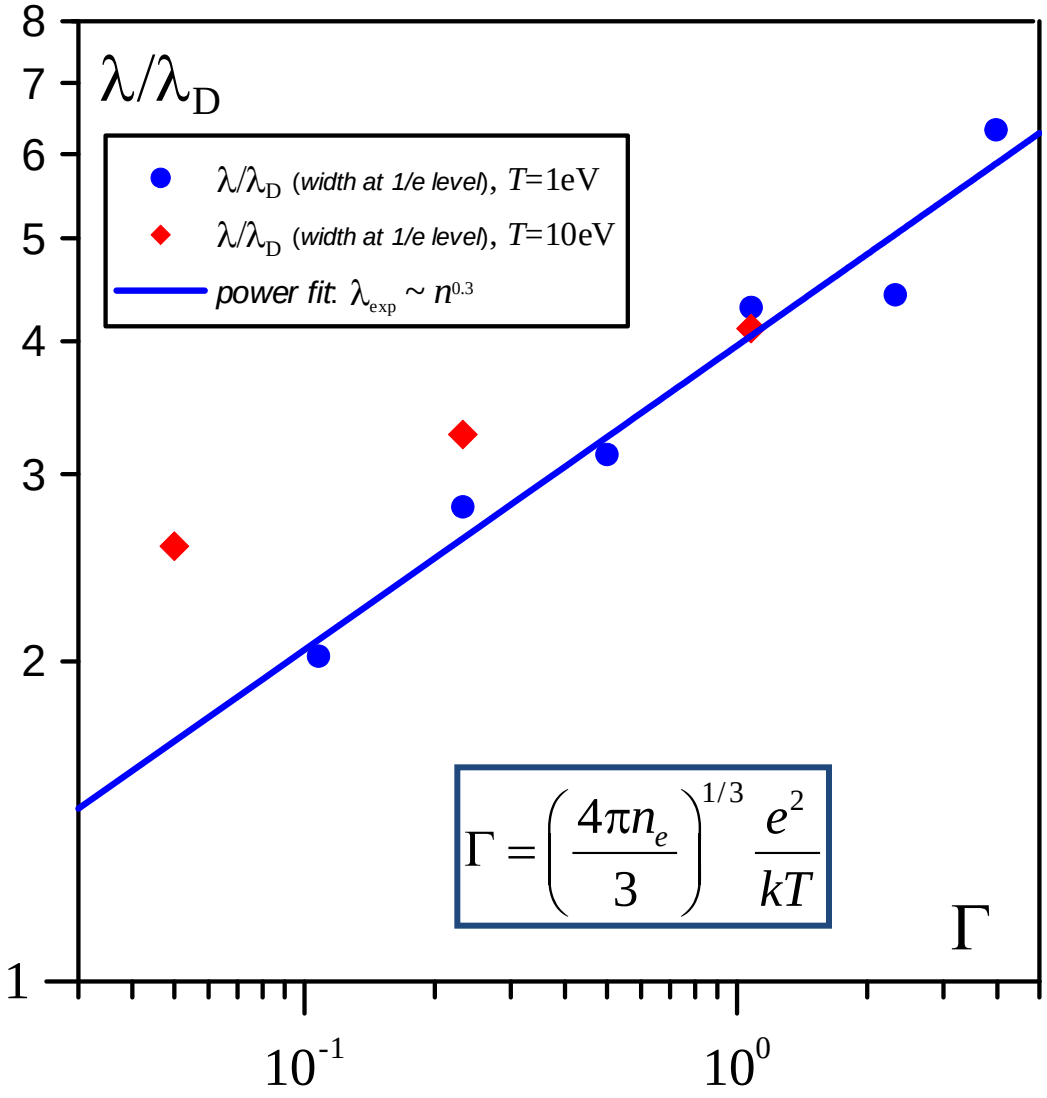
Screening length vs density



Screening length vs density

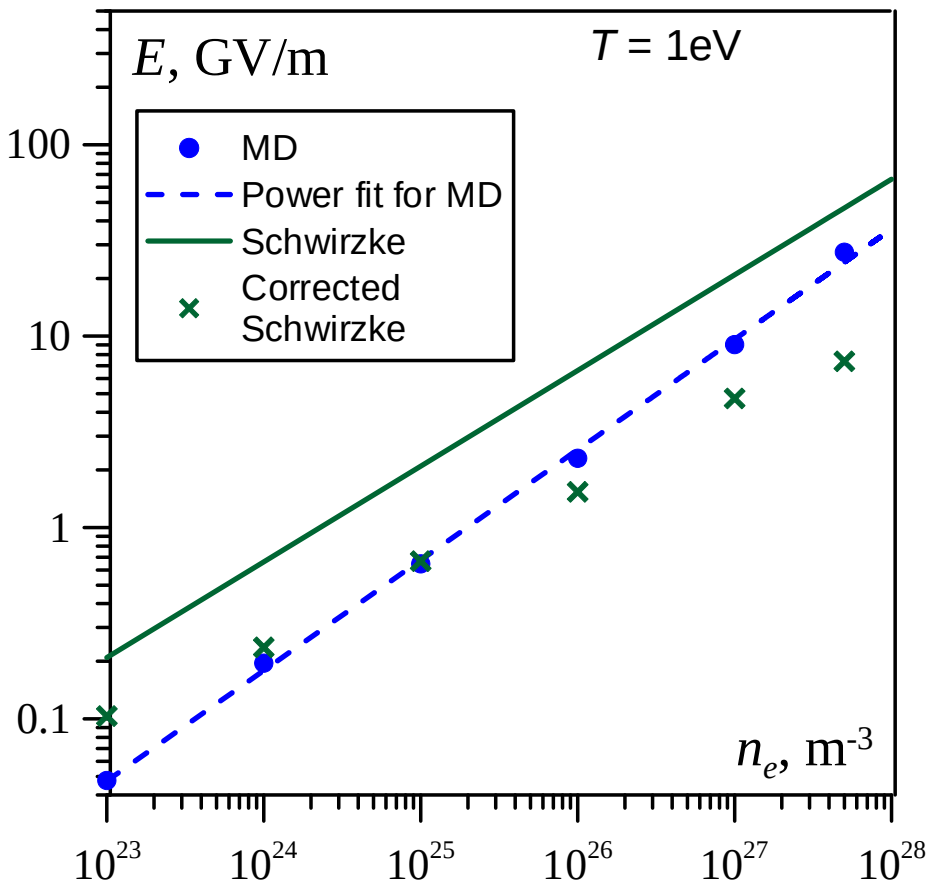


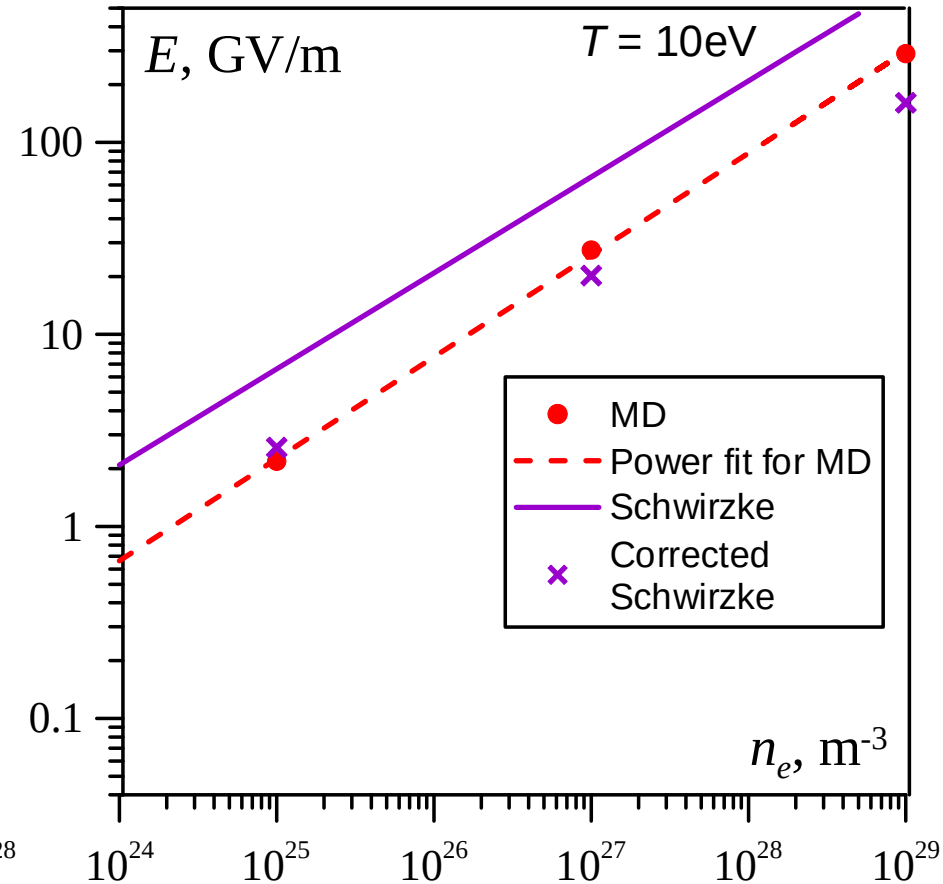
Screening length vs G



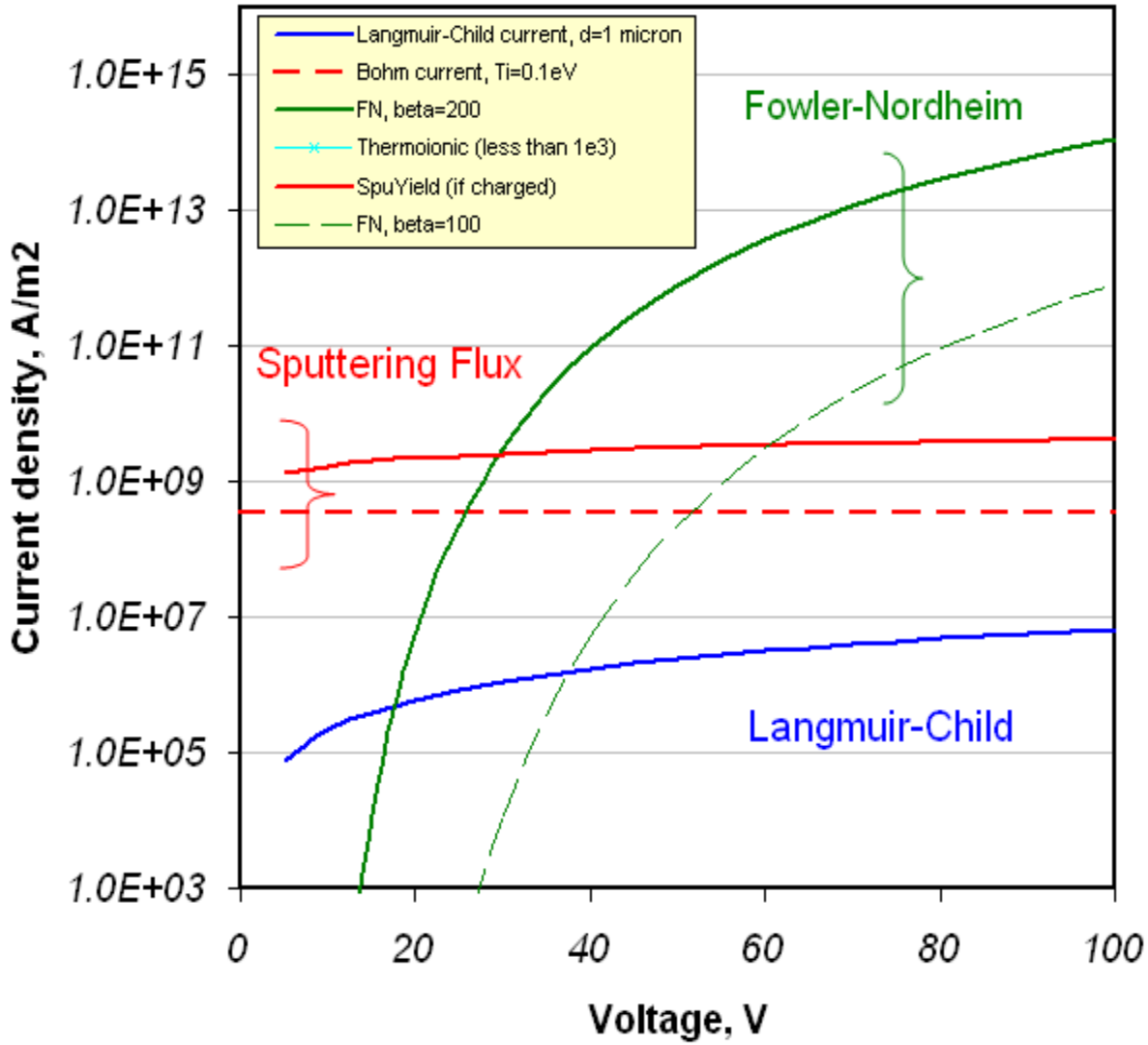
$$\Gamma = \left(\frac{4\pi n_e}{3}\right)^{1/3} \frac{e^2}{kT}$$

E-field vs plasma density





Plasma model of RF breakdown



(1) Fowler-Nordheim equation for electrons (β = 100, 200)

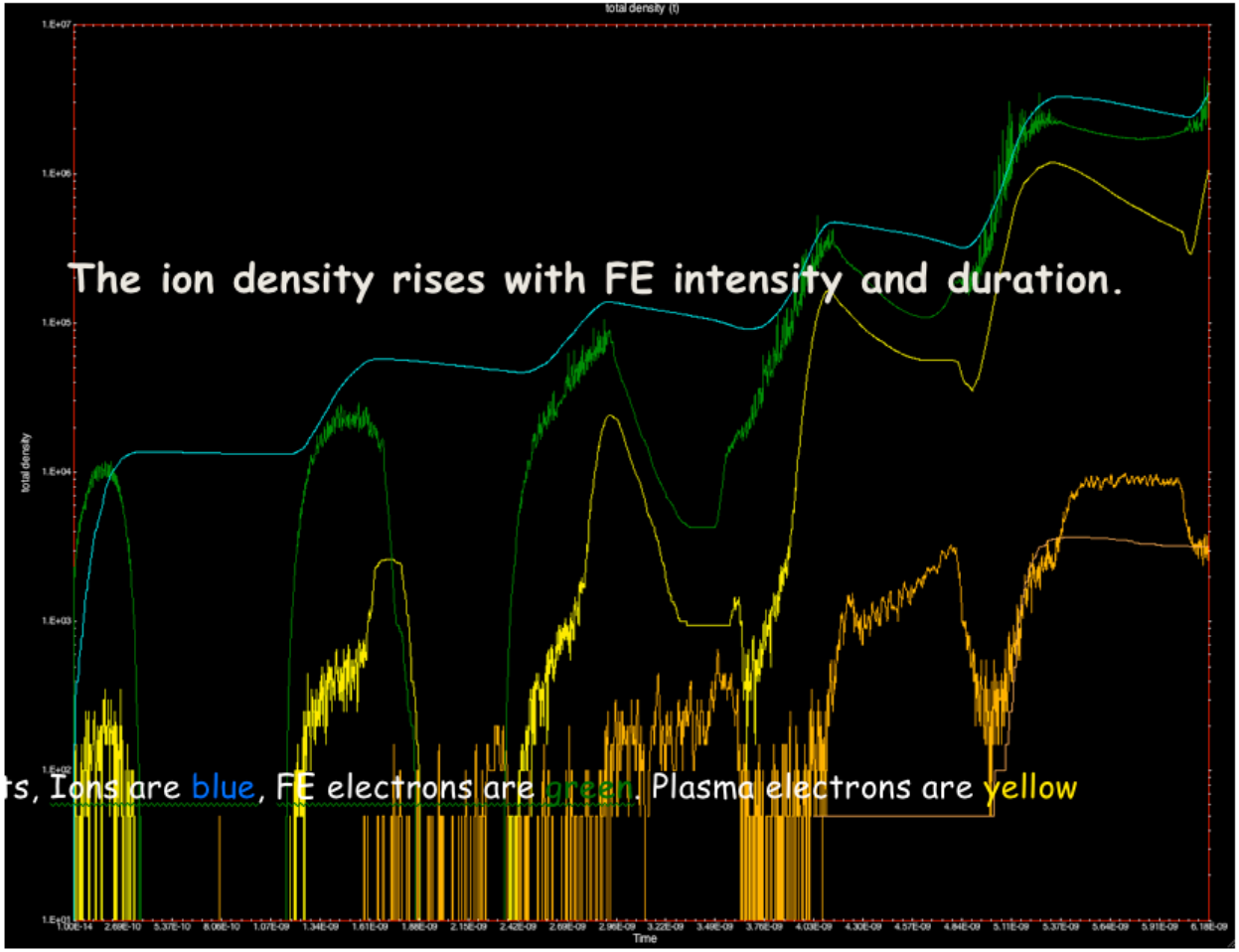
(2) Langmuir-Child equation for ion current from plasma to the tip (*d*=1 μm)

(3) Richardson-Dushman equation for thermionic emission of electrons from liquid Cu (T=1300K)

(4) Sputtering Flux was calculated from Bohm current (plasma ion fluxes) times the sputtering yield at T=1300K

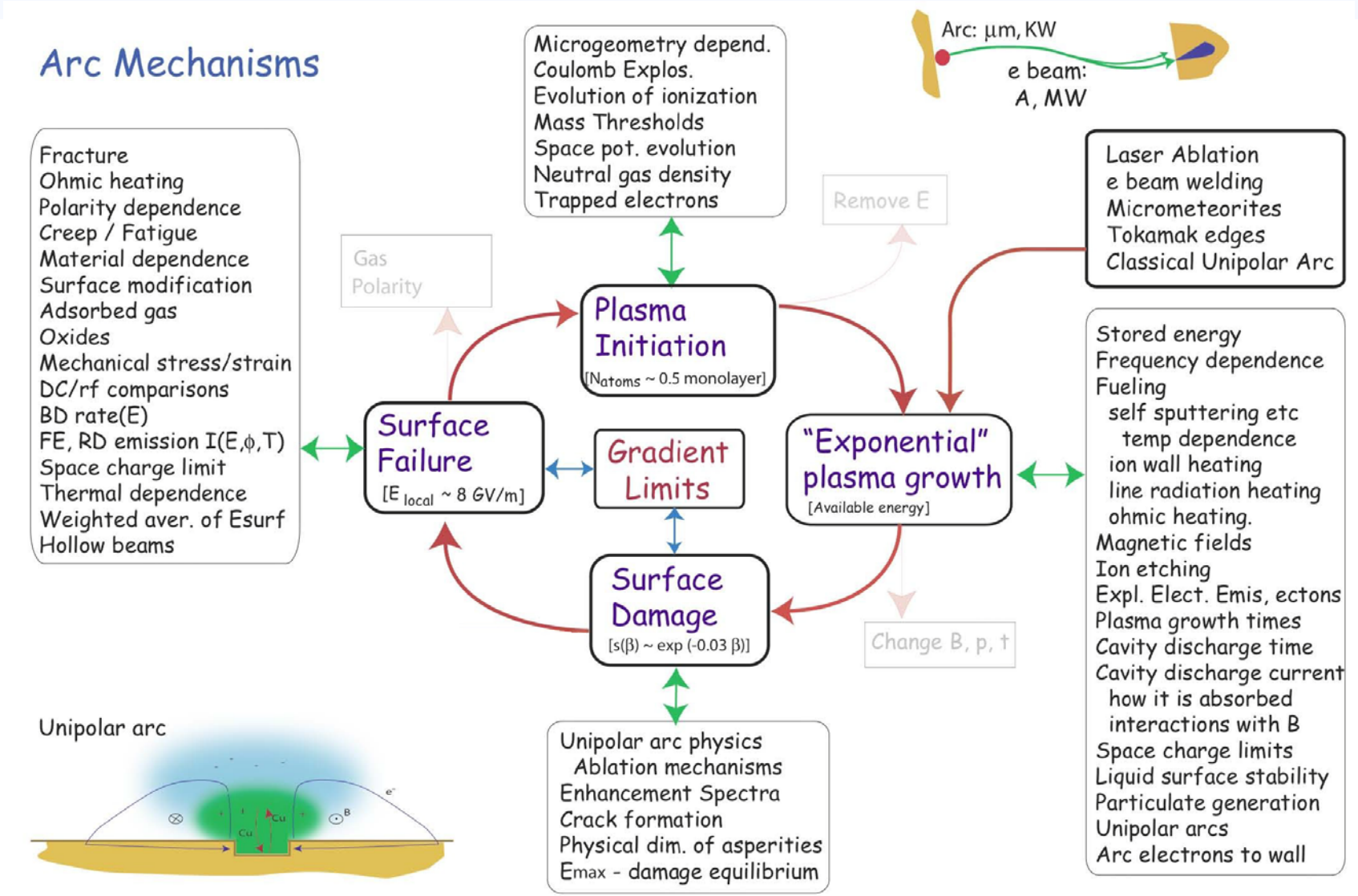
OOPIC Pro 2.5D modeling

Simulation showing how rf arcs start (805 MHz)



In plots, Ions are blue, FE electrons are green, Plasma electrons are yellow

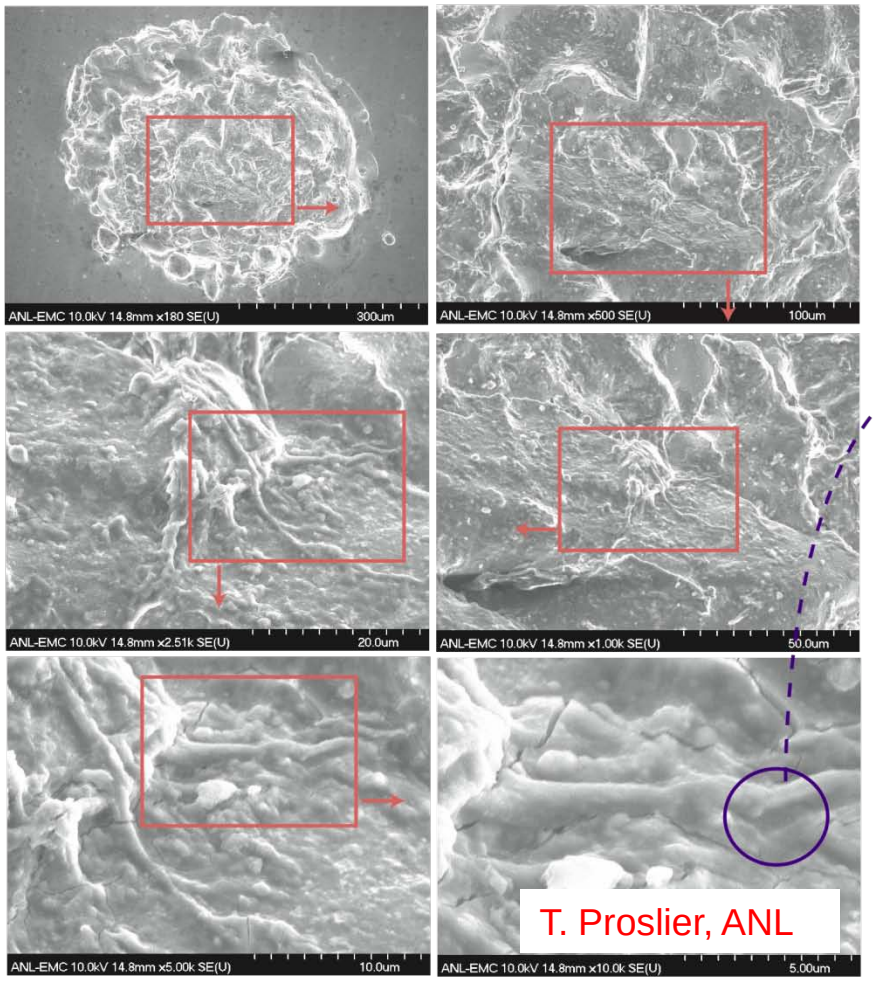
Summary of the Arc model

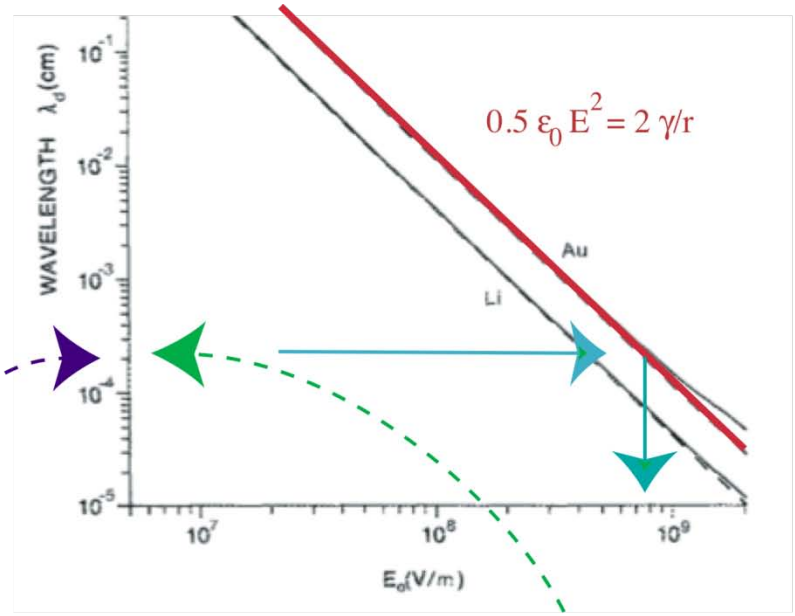


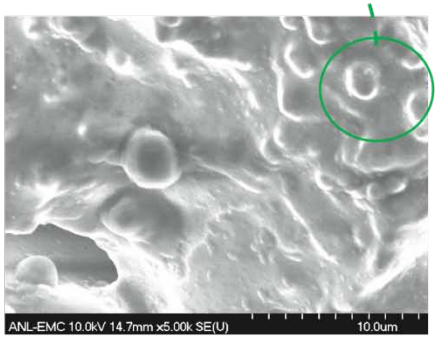
Tonks-Frenkel instability

Capillary waves can measure surface fields

- **Dimensions of structures imply $E_{surface}$ ~ 1 GV/m, if $P_{surface\ tension} = P_{Electrostatic}$.**







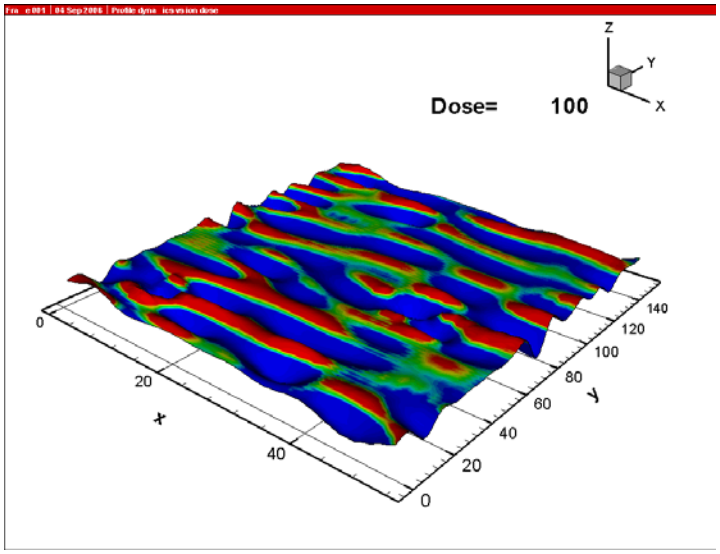
Theory of Thonks instability

The dynamics of a non-equilibrium surface profile in contact with plasma can be determined from an surface dynamics (Kuramoto-Sivashinski) equation:

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

Here, *h* – is the heights at a 2d-position *r* {x,y}, at time *t*.

The coefficients in this equation have the meanings:
η – the viscosity coefficient,
ν – the surface tension term,
***k* - the diffusion coefficient,**
f_{MC} – the sputter by plasma ions.



Other applications of arcing

- We are beginning to develop parameter sets for these cases:
- Tokamak edge plasmas
- Large surface area and long DC pulses.

  This model predicts that breakdown will occur when the E_{local} >5 – 6 GV/m.
- $(\phi/\lambda_D)\beta$ ~ 6 GV/m
- With a 100 eV sheath potential, and λ_D ~ 6 μm gives,
- β ~ (6 GV/m)(6E-6m)/(100 eV) ~ 400,
- Laser Ablation, micrometeorite impacts
- Tiny areas and very short DC pulses.
- Dense plasmas can appear and arcs must trigger more quickly.

  With $\lambda_D \sim 0.1$ μm,
- $(\phi/\lambda_D)\beta$ ~ 11 GV/m,
- ϕ ~ (11 GV/m)(1E-7m)/30 ~ 40 eV
- These arcs would have similar parameters and would develop as described above

Conclusions

- Our picture of arcs is becoming simpler and more general.
- We find electrostatic fields can both trigger and drive arcs.
- Materials properties are the clue for understanding of unipolar arc formation and rf breakdown.
- We are exploring new mechanisms and news models, with a number of papers underway.