Field emission assisted heating of Cs2Te photocathode: Implication toward mesoscale surface breakdown

Ryo Shinohara

LANL Mentors: Danny Perez, Soumendu Bagchi
MSU Advisor: Sergey Baryshev
CARIE Project team: Evgenya Simakov, Chengkun Huang, etc.

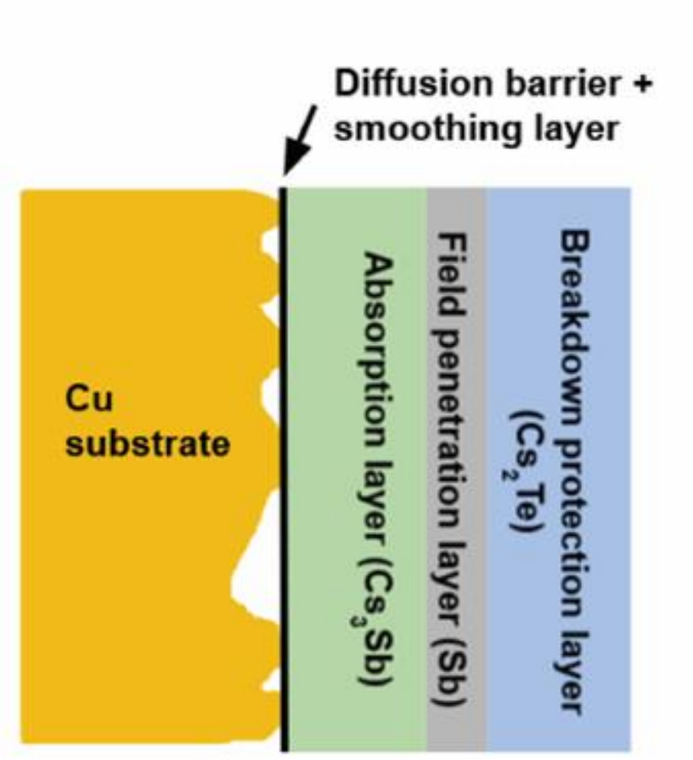
Overview

- **CARIE Project**
  - **Theory effort**
- Mesoscale Surface Diffusion Model
- Field Emission Modeling
- Result
- Conclusion / Future Work

CARIE: Cathodes And Rf Interactions in Extremes

A new three-year project was funded at LANL to demonstrate operation of high-quantum-efficiency cathodes in a high-gradient RF injector.

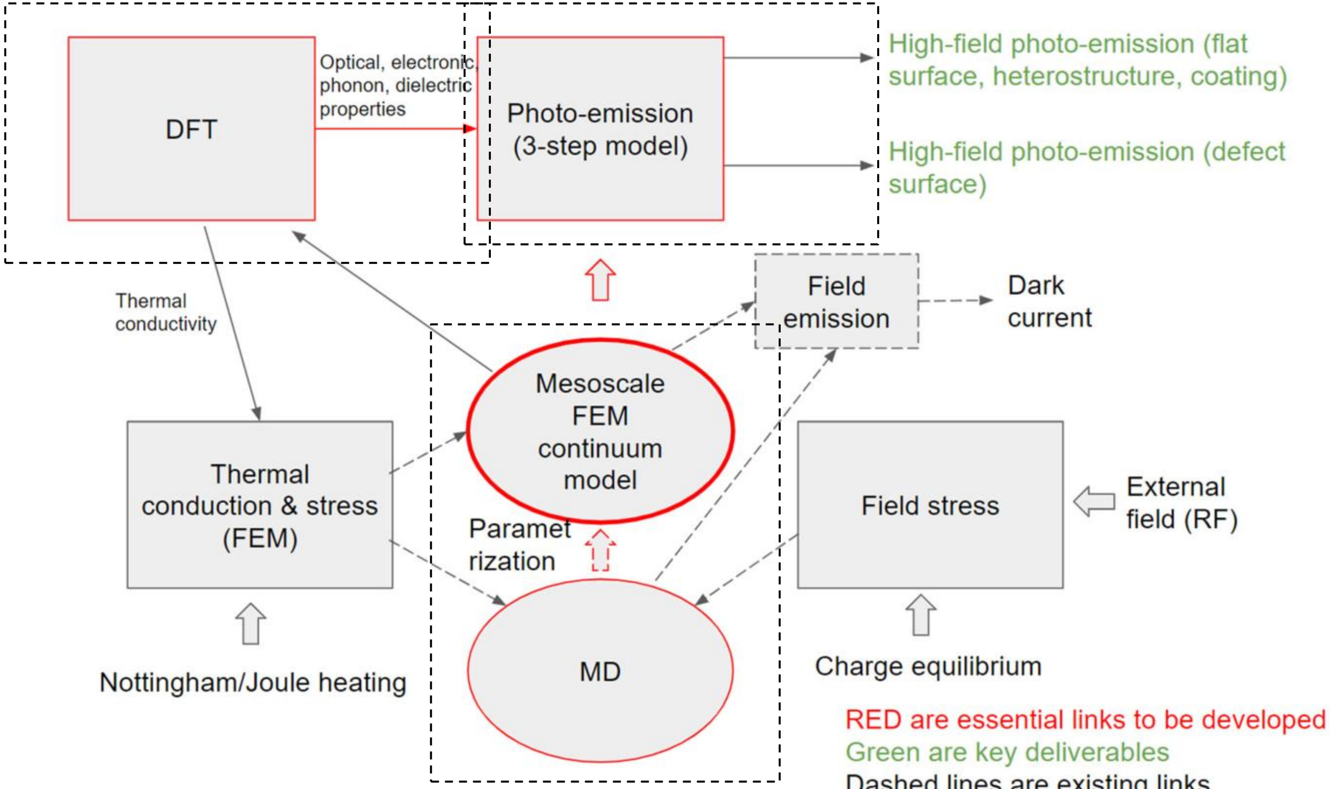
- Project builds upon LANL's expertise in high-gradient C-band and high-QE photocathodes.
- The proposed heterostructured cathode will include multiple layers to ensure atomic flatness of the surface, high QE, and the ability to withstand high electric fields with no breakdown.
- Target beam parameters: 250 pC, 0.1 µm*rad, $B_{5D} = 10^{16}$ A/m^2.
- The project started in October of 2022.



Theory efforts: thrusts and the team

- New photoemission model for thin-film semiconductor cathodes (D. Dimitrov)
- DFT modeling of cathode materials (Cs_2Te and Cs/alkaline antimonides) (G. Wang)
  - Bulk properties (structure, optical, electronic, photon, and atomic potential)
  - Surface properties (work function, electronic properties)
- Monte-Carlo (MC) high-field transport modeling (C. Huang, D. Dimitrov)
- Molecular Dynamics (MD) models for cathode materials (S. Bagchi, D. Perez)
  - Beyond standard charge equilibration approach for high-field operation
  - Data-driven parametrization of interatomic potentials
- **Meso-scale surface breakdown modeling** (S. Bagchi, R. Shinohara - MSU)
- Integration of the nano/meso-scale models

Overview of our models and the integrated modeling approach for semiconductor cathodes



RED are essential links to be developed

Green are key deliverables

Dashed lines are existing links

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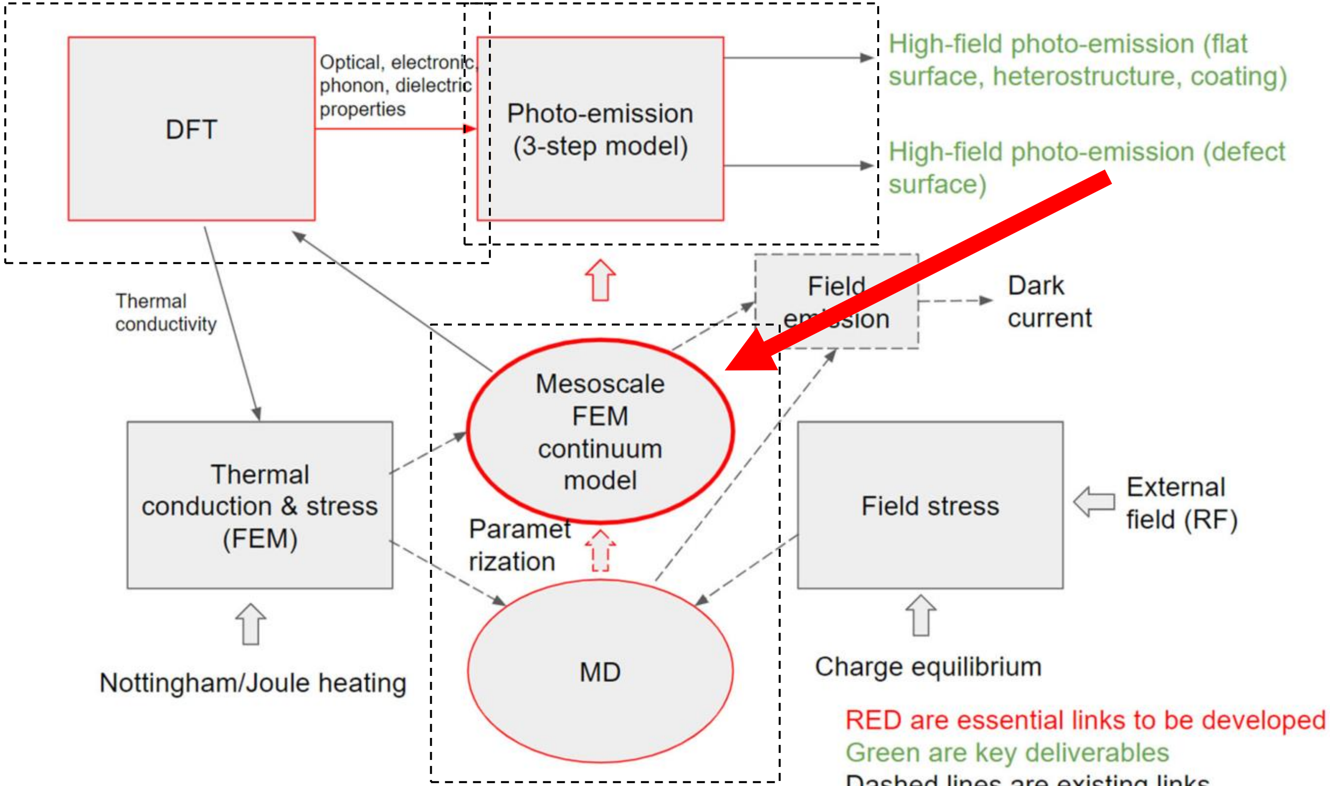

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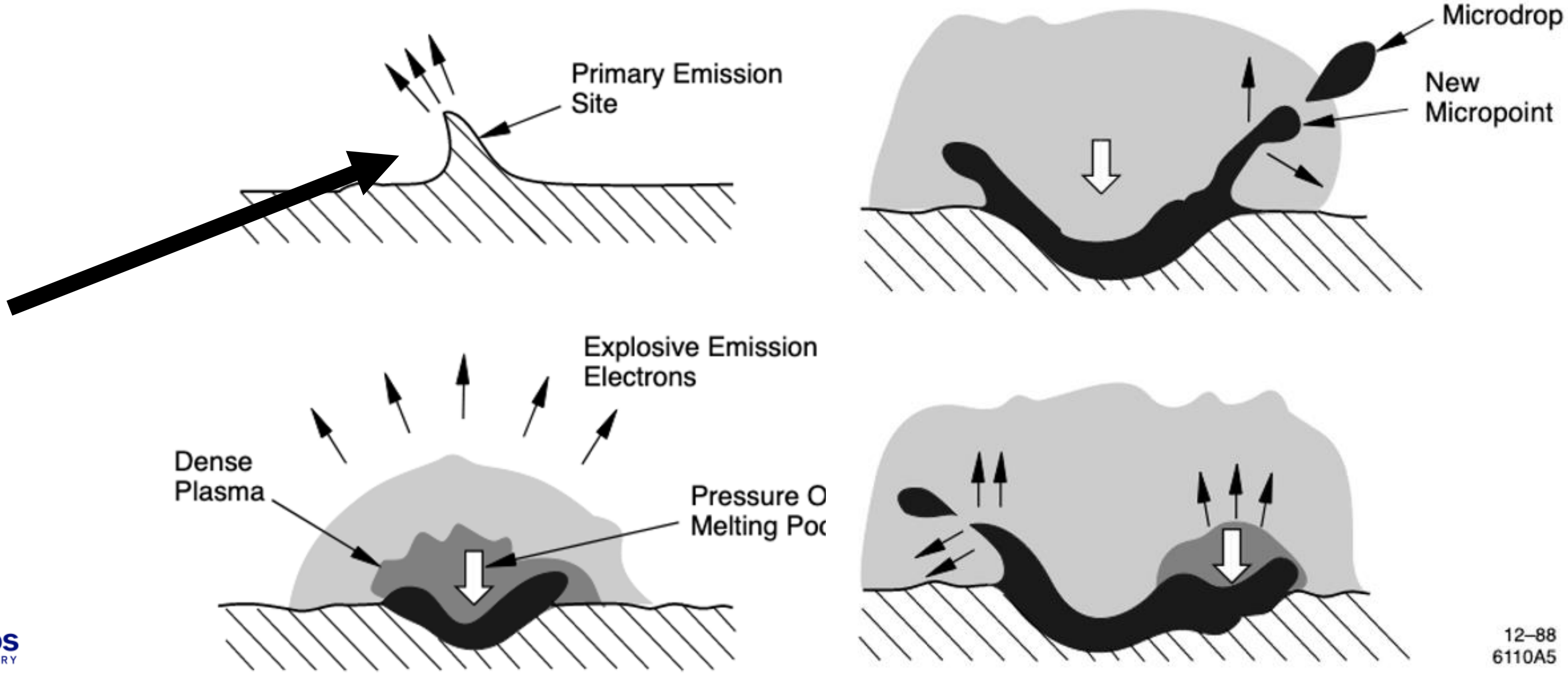
Breakdown Under High Field Environment

- Triggered from primary emission site

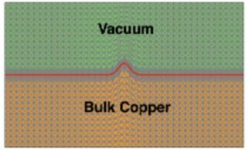
Wang JW, Loew GA (1997)



Mesoscale Surface Diffusion Model

①

Finite Element Method



1. Local field distribution is solved on the vacuum mesh
2. Linear Thermoelasticity is solved on the copper mesh

② & ③

Linear Thermoelasticity

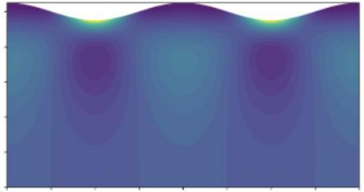
$$-\nabla \cdot \sigma(u) = 0$$

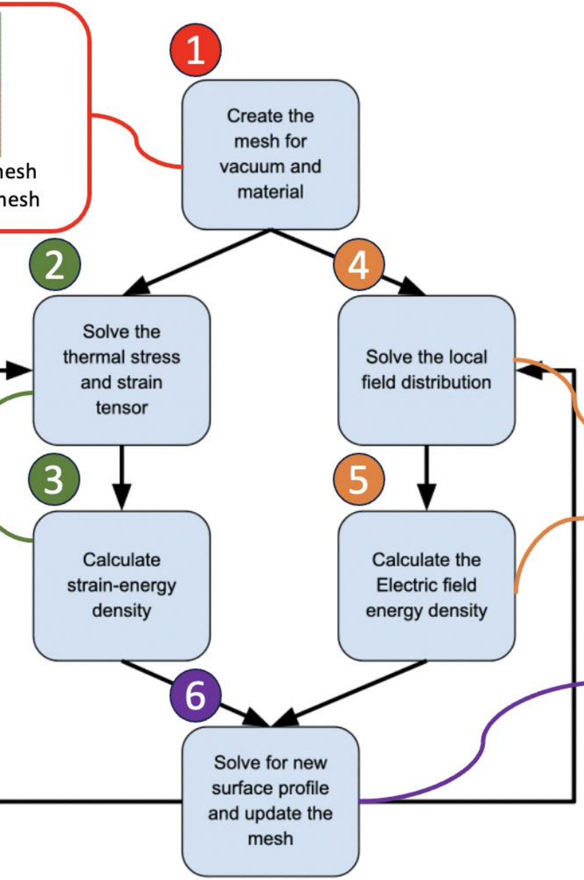
$$\sigma(u) = \lambda tr(\epsilon(u))\mathbb{1} + 2\mu\epsilon(u) - \frac{\alpha Y}{1-2\nu}\Delta T\mathbb{1}$$

$$\epsilon(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$$

Strain-Energy Density

$$\omega_T = \frac{1}{2}\sum_i^2\sum_j^2 \sigma_{ij}\epsilon_{ij} = \frac{1}{2}\begin{pmatrix} \sigma_{11}\epsilon_{11} + \sigma_{22}\epsilon_{22} \\ +\sigma_{12}\epsilon_{12} + \sigma_{21}\epsilon_{21} \end{pmatrix}$$





① Create the mesh for vacuum and material

② Solve the thermal stress and strain tensor

③ Calculate strain-energy density

④ Solve the local field distribution

⑤ Calculate the Electric field energy density

⑥ Solve for new surface profile and update the mesh

④ & ⑤

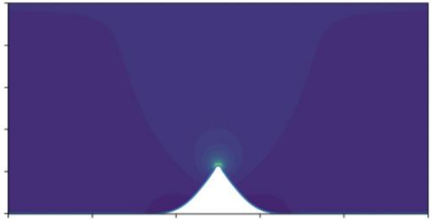
Electrostatic

$$\nabla \cdot (\nabla\phi) = 0$$

$$E = -\nabla\phi$$

Field Energy Density

$$U_E = \frac{1}{2}\epsilon_0 E^2$$



⑥

Surface Diffusion

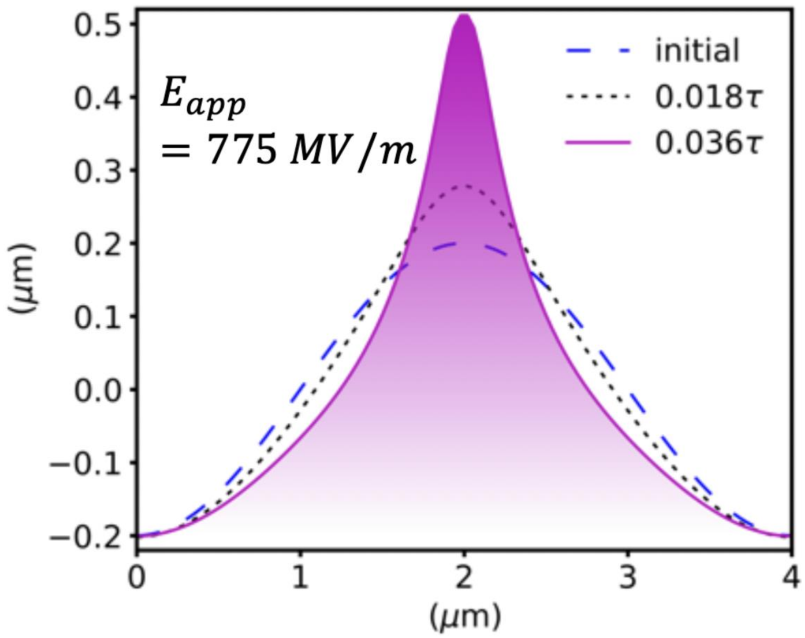
$$V_n = \frac{D_s\Omega v_s}{k_b T}\frac{\partial^2\mu_c}{\partial s^2}$$

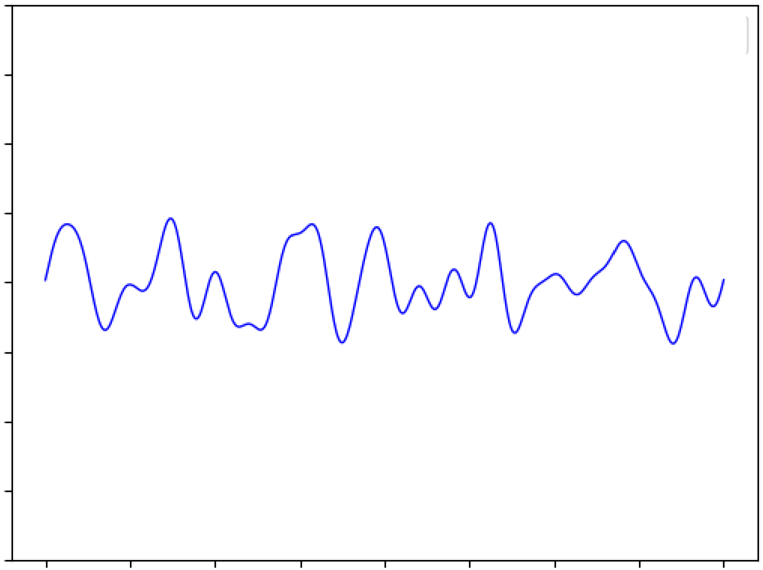
$$\frac{\partial h}{\partial t} = \frac{D_s v_s \Omega}{k_B T}\frac{\partial}{\partial x}[(1+h_x')^{-1/2}\frac{\partial}{\partial x}(\mu_c)]$$

$$\mu_c = \Omega(\gamma k - U_E + \omega_T)$$

Chemical potential = surface tension + electrostatic energy + strain energy density

Mesoscale surface diffusion model





https://arxiv.org/pdf/2311.06624.pdf
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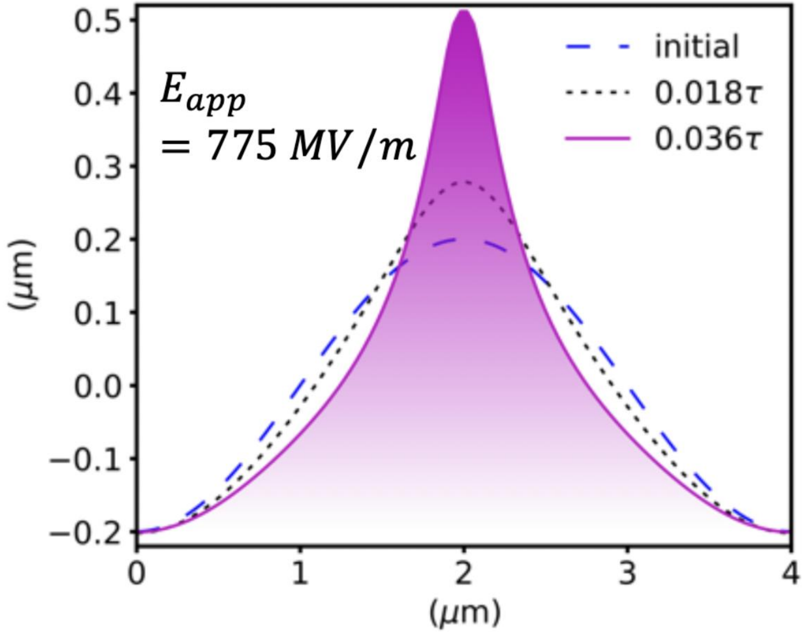

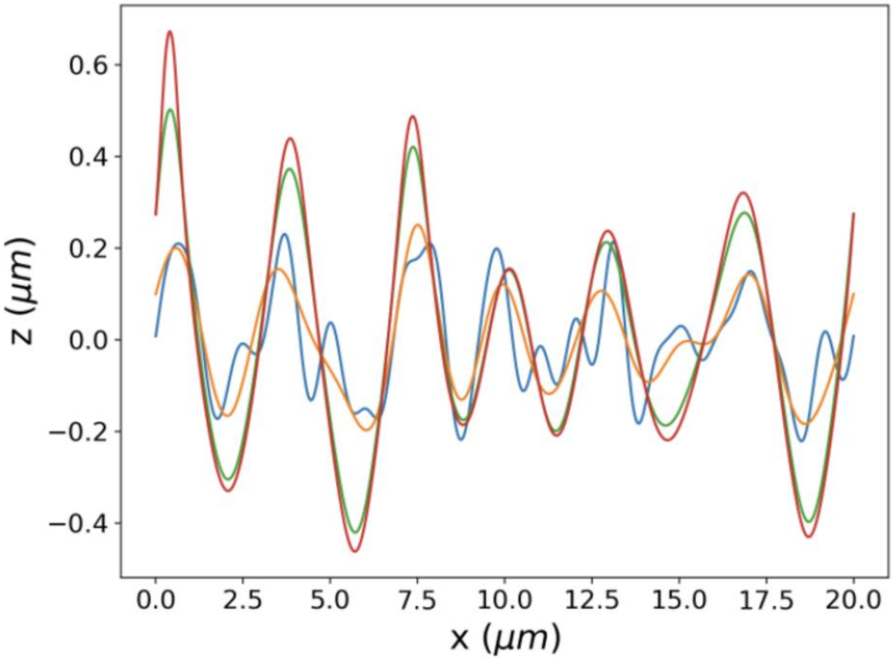

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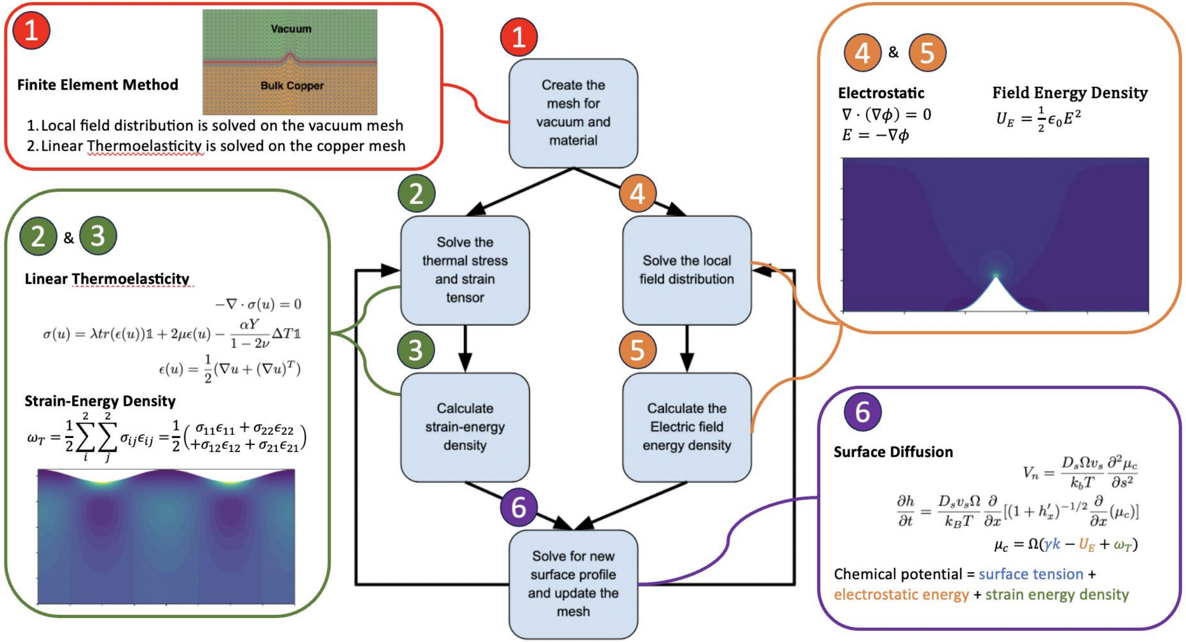
Semiconductor Breakdown: Field Emission

- Field Emission
  - Source → Current Density
    - Joule Heating
    - Nottingham Effect



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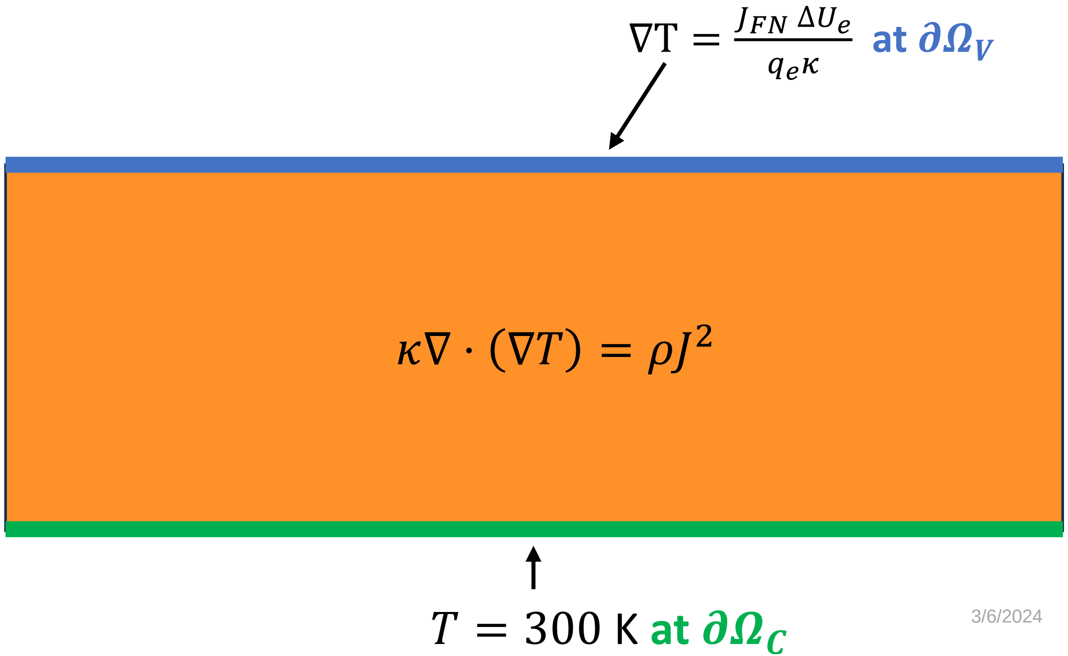
$$\mu_c = \Omega(\gamma k - U_E + \omega_T)$$

Chemical potential = surface tension + electrostatic energy + strain energy density

Field Emission Current & Heating

- Field Emission Calculated through Fowler-Nordheim equation
  - $J_{FN} = 1.54 * 10^6 * 10^{4.53\phi^{-0.5}}[E_{local}]^2 Exp(\frac{-6.53*10^9*\phi^{1.5}}{E_{local}})$
- Joule heating:
  - $\frac{\partial T}{\partial t} = \rho \boldsymbol{J}_{\boldsymbol{bulk}}^{\boldsymbol{2}}$
- Nottingham Heating:
  - $\nabla T \cdot \vec{n} = \frac{J_{FN} \Delta U_e}{q_e \kappa}$



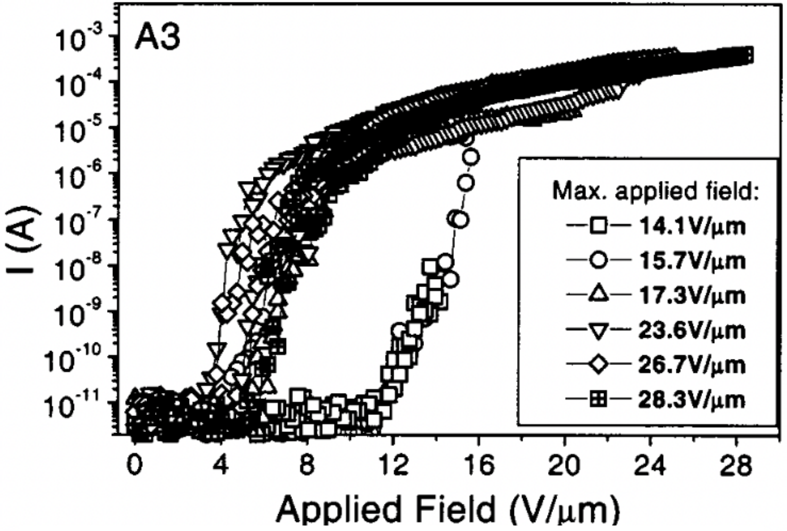
$\nabla \mathrm{T} = \frac{J_{FN}\,\Delta U_e}{q_e \kappa}$ **at $\partial\Omega_V$**

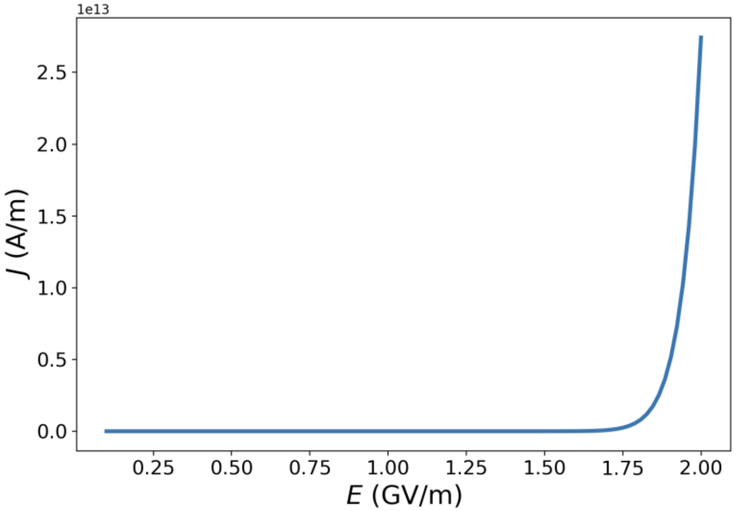
$$\kappa \nabla \cdot (\nabla T) = \rho J^2$$

$T = 300$ K **at $\partial\Omega_C$**

Deviation from FN equation for semiconductor

- Current-density Saturation in semiconductor
- Strong Deviation from classical FN equation in high-field regime
  - $1.54*10^{6}*10^{4.53\phi^{-0.5}}[\boldsymbol{E_{local}}]^{2}Exp(-\frac{6.53*10^{9}*\phi^{1.5}}{\boldsymbol{E_{local}}})$
  - FN equation predicts that current increases exponentially with surface field





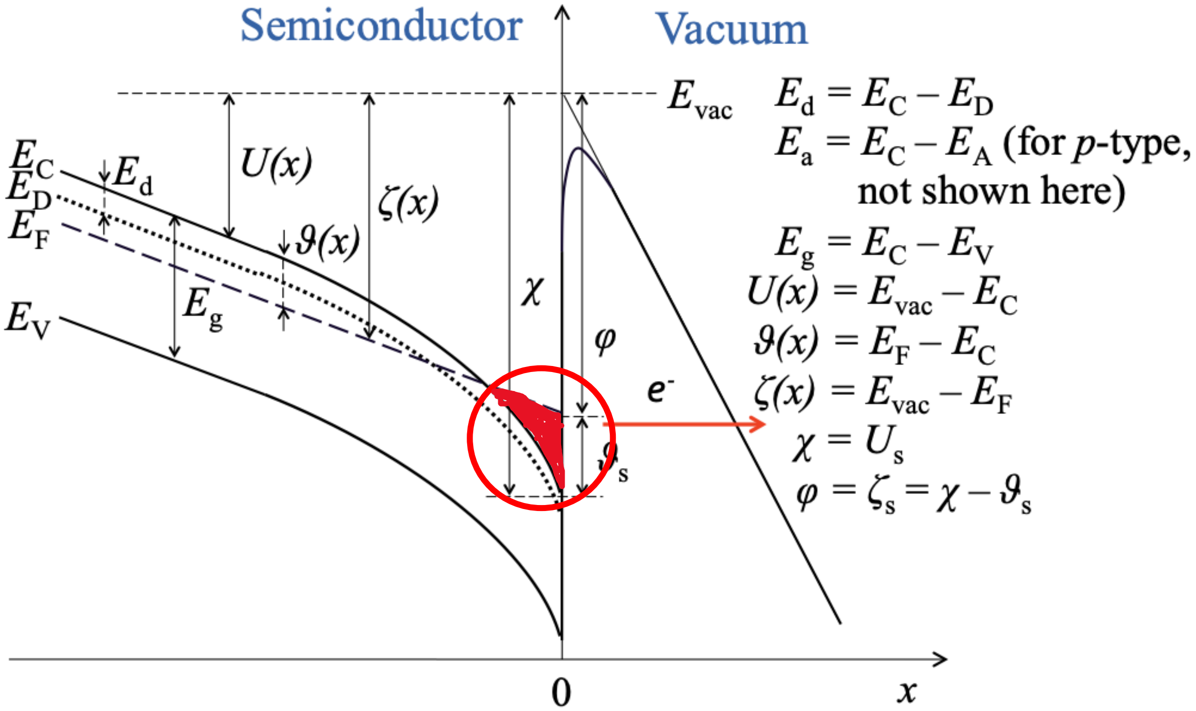
Journal of Applied Physics **125**, 205303 (2019); https://doi.org/10.1063/1.5085679

Un-physical results with FN equation

- Temperature Rise per Applied Field for Joule Heating:
  - 100MV/m: ~0°K
  - 125MV/m ~0 °K
  - **150MV/m: ~12 °K**
  - **175MV/m: ~14000 °K**
- Temperature Rise per Applied Field for Notting
  - 50MV/m: ~0°K
  - 55MV/m ~1 °K
  - **60MV/m: ~180 °K**
  - **65MV/m: ~16000 °K**

Unrealistic Temperature Spike

Stratton-Baskin-Lvov-Fursey Formalism, Oksana Chubenko



$$E_d = E_C - E_D$$
$$E_a = E_C - E_A \text{ (for } p\text{-type, not shown here)}$$
$$E_g = E_C - E_V$$
$$U(x) = E_{vac} - E_C$$
$$\vartheta(x) = E_F - E_C$$
$$\zeta(x) = E_{vac} - E_F$$
$$\chi = U_s$$
$$\varphi = \zeta_s = \chi - \vartheta_s$$

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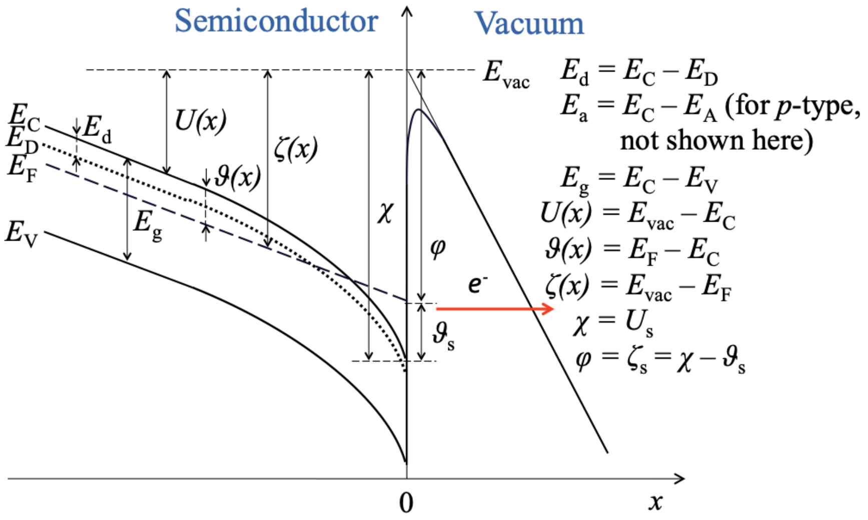
Stratton-Baskin-Lvov-Fursey Formalism, Oksana Chubenko

- Low-field Regime
  - Limited by tunneling probability
  - → Act metal like (follows FN)
- High-field Regime (saturation)
  - Limited by electron supply in the space-charge (band-bending) region
- Formalism takes into account the band-bending



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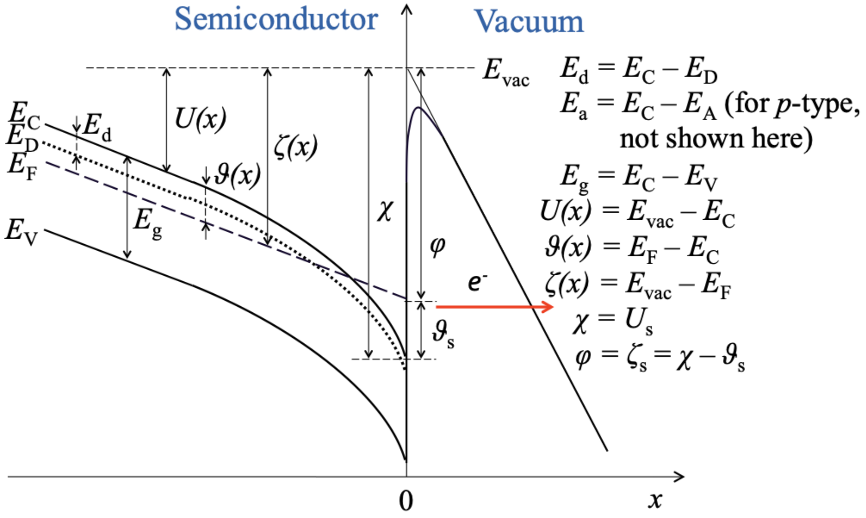

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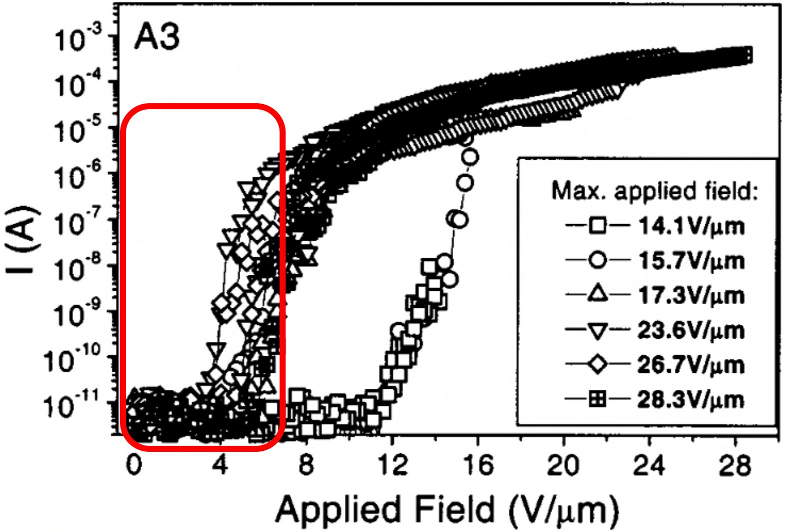

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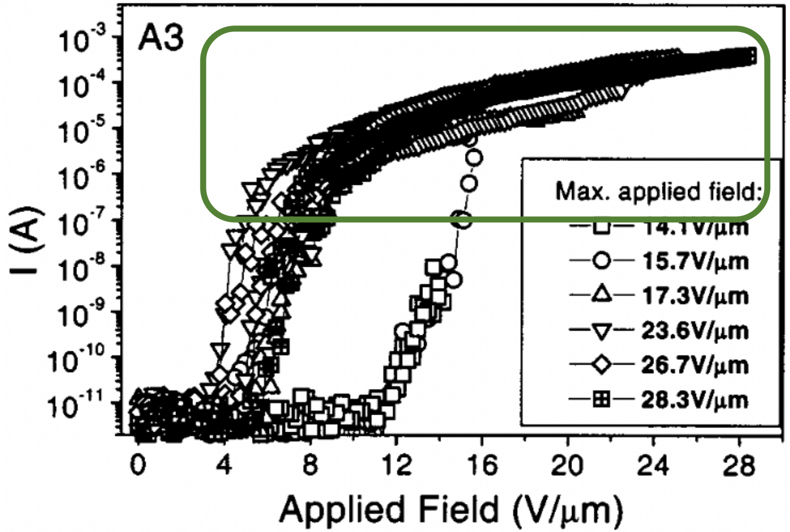

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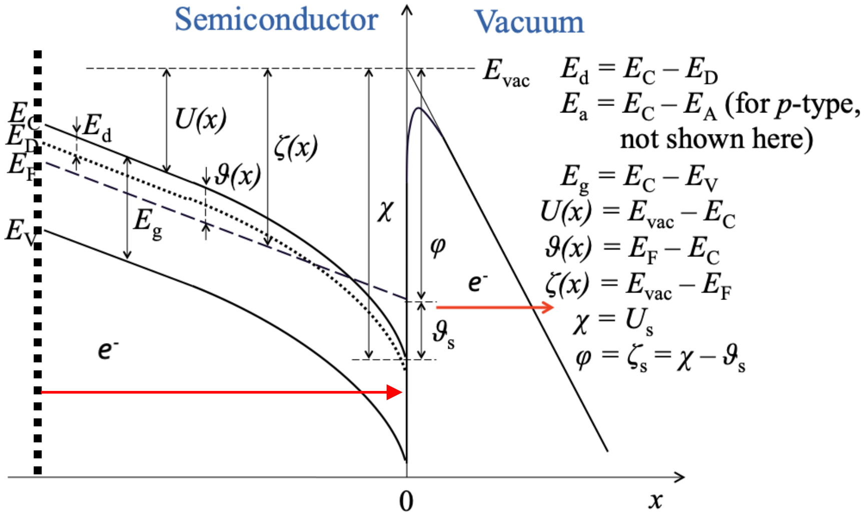

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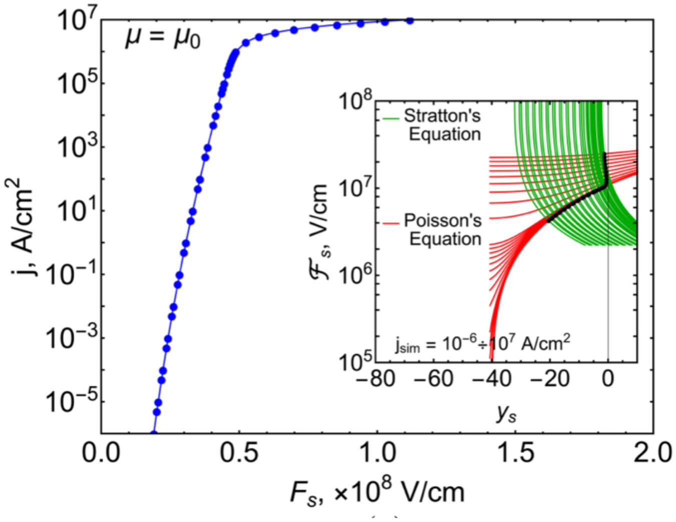
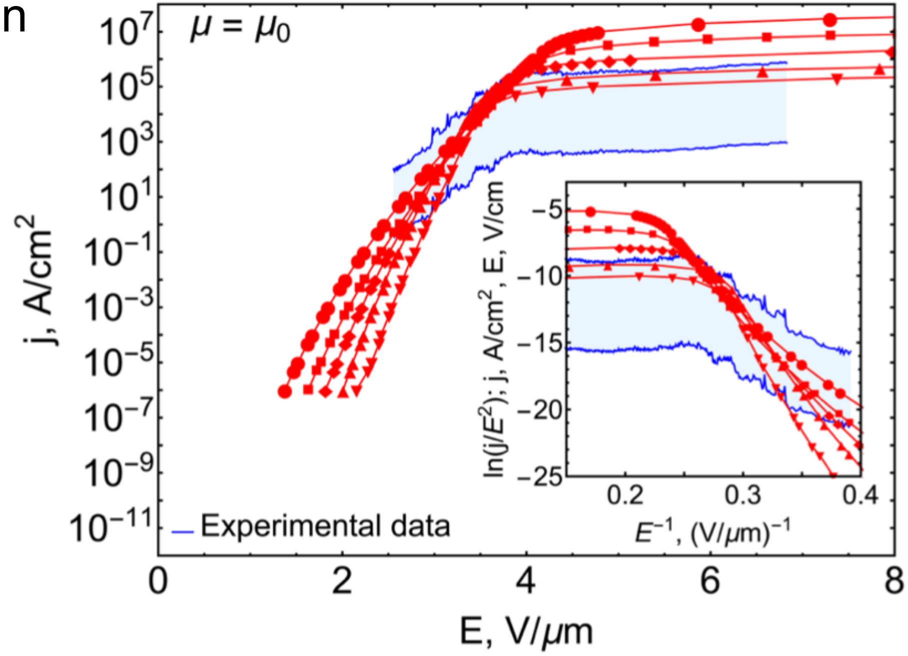
Stratton-Baskin-Lvov-Fursey Formalism

- Find the simultaneous solution of the Poisson equation and Stratton's equation
- Oksana Chubenko studied (N)UNCD





Poisson Equation

- Solve

$$-\frac{d^2V}{dx^2} = -\frac{\rho}{\kappa\epsilon_0}, \rho = -q(n - p + N_a^- - N_d^+)$$

$$\boxed{y(x) \equiv \frac{\vartheta(x)}{k_\mathrm{B}T} = \frac{E_\mathrm{F} - E_\mathrm{C}}{k_\mathrm{B}T}.}$$

Concentration Densities

$$\left\{\begin{aligned} n &= N_\mathrm{C}F_{1/2}[(E_\mathrm{F} - E_\mathrm{C})/k_\mathrm{B}T], \\ p &= N_\mathrm{V}F_{1/2}[(E_\mathrm{V} - E_\mathrm{F})/k_\mathrm{B}T], \\ N_\mathrm{a}^- &= \frac{N_\mathrm{a}}{1 + 2\exp\left[(E_\mathrm{A} - E_\mathrm{F})/k_\mathrm{B}T\right]}, \\ N_\mathrm{d}^+ &= \frac{N_\mathrm{d}}{1 + 2\exp\left[(E_\mathrm{F} - E_\mathrm{D})/k_\mathrm{B}T\right]}, \end{aligned}\right.$$

$$\begin{aligned} n(y) &= N_\mathrm{C}F_{1/2}(y), \\ p(y) &= N_\mathrm{V}F_{1/2}(-E_\mathrm{g}/k_\mathrm{B}T - y), \\ N_\mathrm{a}^-(y) &= \frac{N_\mathrm{a}}{1 + 2\exp\left(-E_\mathrm{a}/k_\mathrm{B}T - y\right)}, \\ N_\mathrm{d}^+(y) &= \frac{N_\mathrm{d}}{1 + 2\exp\left(E_\mathrm{d}/k_\mathrm{B}T + y\right)}. \end{aligned}$$

Stratton’s Equation

$$j_{\mathrm{em}}^{-}(F_{\mathrm{s}}, y_{\mathrm{s}}) = A_1 \exp\left[-B_1 \frac{\chi^{3/2}}{F_{\mathrm{s}}} v(Y_1)\right] \exp\,(y_{\mathrm{s}}) \times \left[1 - C_1 \frac{\chi^{1/2}}{F_{\mathrm{s}}} t(Y_1) k_{\mathrm{B}} T\right]^{-1},$$

$$j_{\mathrm{em}}^{+}(F_{\mathrm{s}}, y_{\mathrm{s}}) = \frac{A_2}{t^2(Y_2)} \frac{F_{\mathrm{s}}^2}{\varphi(y_{\mathrm{s}})} \exp\left[-B_1 \frac{\varphi^{3/2}(y_{\mathrm{s}})}{F_{\mathrm{s}}} v(Y_2)\right] \times \left\{1 - \exp\left[-B_2 \frac{\varphi^{1/2}(y_{\mathrm{s}})}{F_{\mathrm{s}}} y_{\mathrm{s}} t(Y_2)\right] \times \left[1 + B_2 \frac{\varphi^{1/2}(y_{\mathrm{s}})}{F_{\mathrm{s}}} y_{\mathrm{s}} t(Y_2)\right]\right\},$$

Parameters	Expression
A_1	$4\pi m_0 q (k_B T)^2 / h^3$
B_1	$8\pi\sqrt{2m_0}/(3qh)$
C_1	$4\pi\sqrt{2m_0}/(qh)$
A_2	$q^3/(8\pi h)$
B_2	$4\pi\sqrt{2m_0} k_B T/(qh)$

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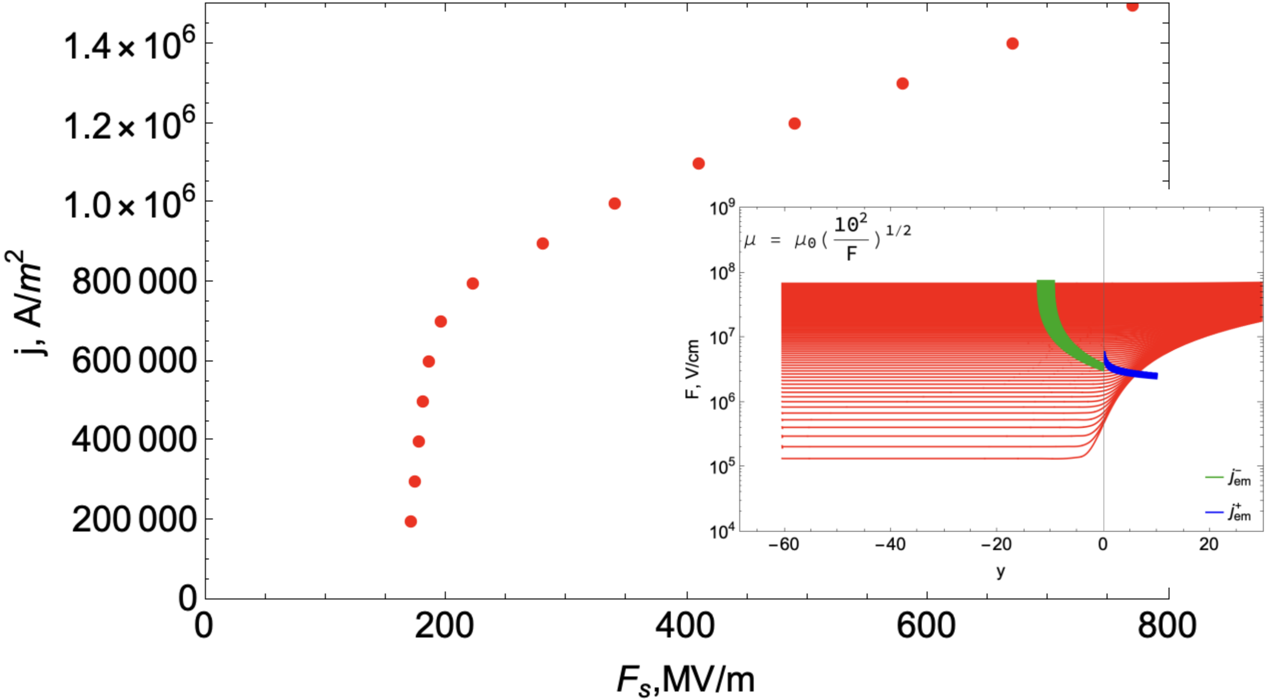
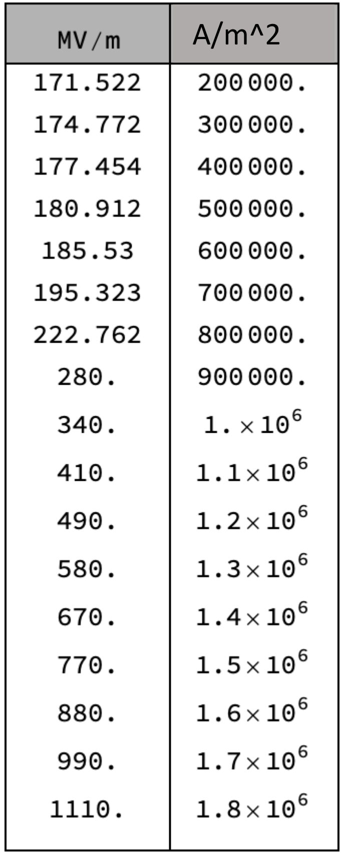
Current vs Field: Current Saturation





MV/m	A/m^2
171.522	200000.
174.772	300000.
177.454	400000.
180.912	500000.
185.53	600000.
195.323	700000.
222.762	800000.
280.	900000.
340.	$1. \times 10^6$
410.	1.1×10^6
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580.	1.3×10^6
670.	1.4×10^6
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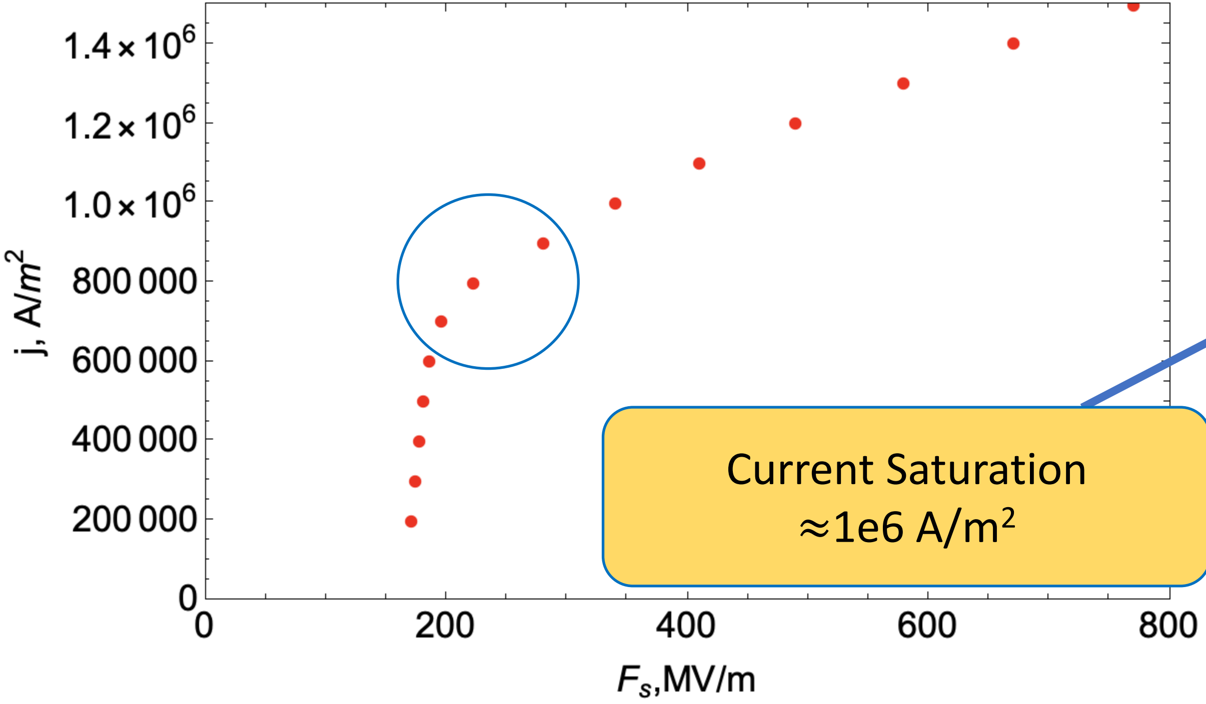
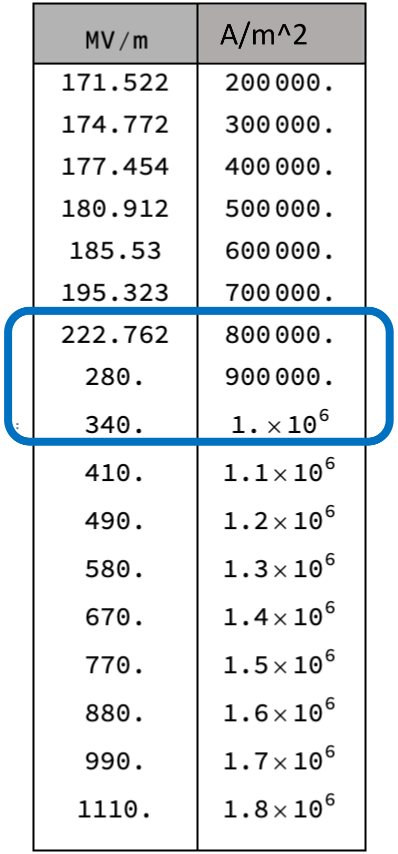


Current Saturation
≈1e6 A/m^2



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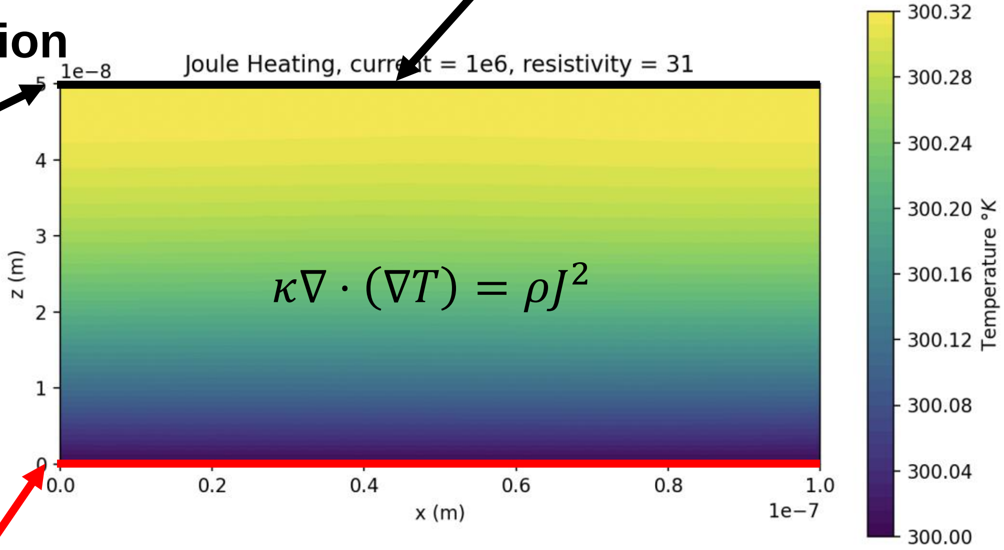
Simple heating test with the solved current

- 50nm thin coat
- Solving for **Stationary Heat Equation**
  - $\kappa\nabla\cdot(\nabla T) = f$
  - Joule Heating:
    - $f = \rho J_{bulk}^2$
  - Nottingham Heating:
    - $\nabla T\cdot\vec{n} = \frac{J_{bulk}\Delta U_e}{q_e\kappa}$
    - $f = \nabla\cdot(\kappa\Delta T)$



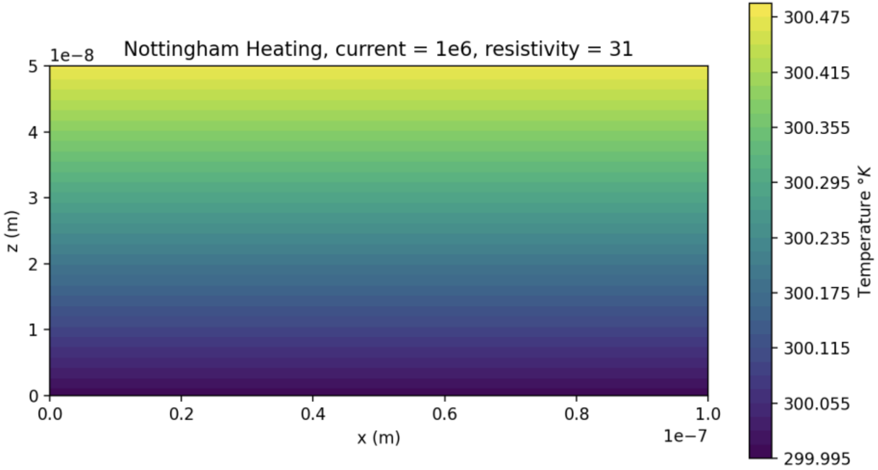
$$\kappa\nabla\cdot(\nabla T) = \rho J^2$$

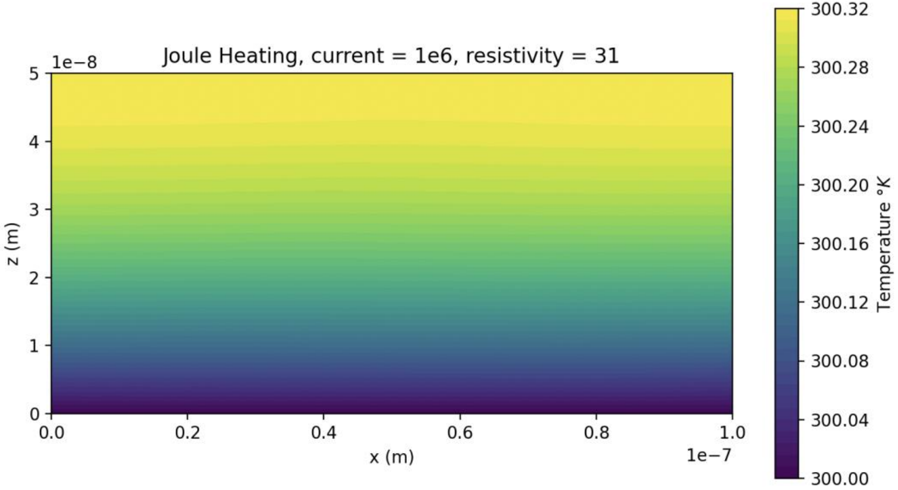
Semiconductor vacuum boundary

Copper semiconductor boundary: $T = 300$ K on $\boldsymbol{\partial\Omega_C}$

Heating: max ΔT

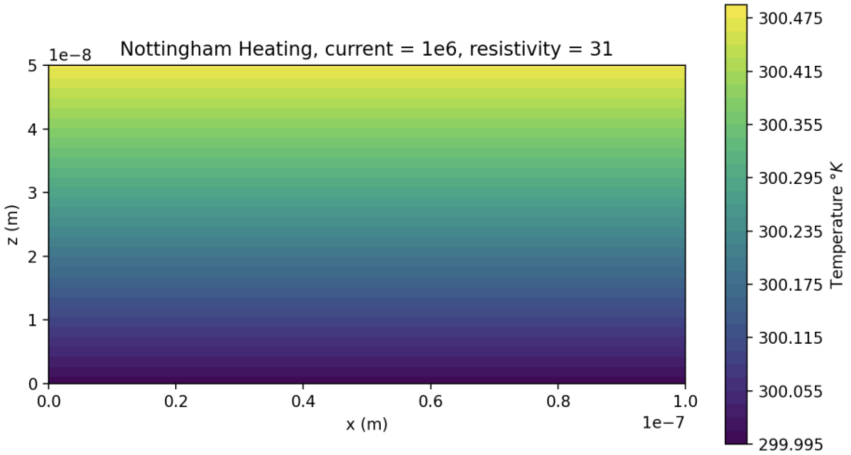
- **Joule Heating $\boldsymbol{\Delta T}$:** $\mathbf{0.32}$ K
- **Nottingham Effect $\boldsymbol{\Delta T}$:** $\mathbf{0.47}$ K

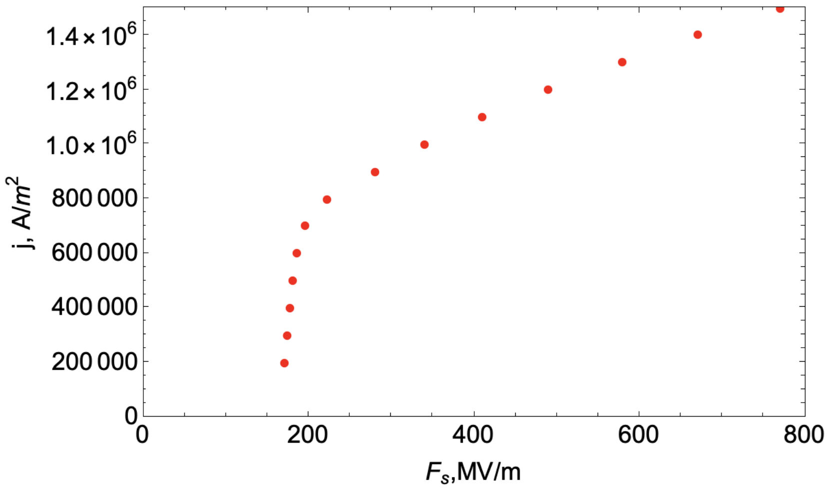


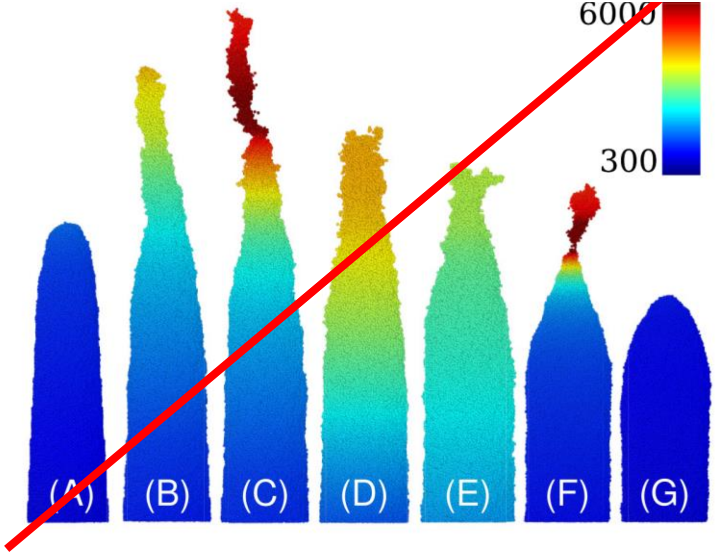


Conclusion

- Current Saturation
- Insufficient current for meaningful heating to take place
  - Max ΔT of 0.8 K
- Thermal Runaway will (likely) to not take place



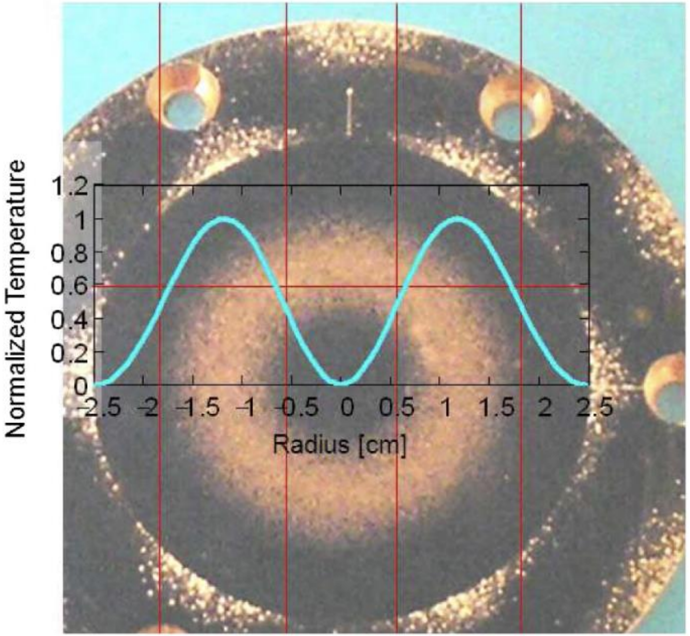




Moving Forward

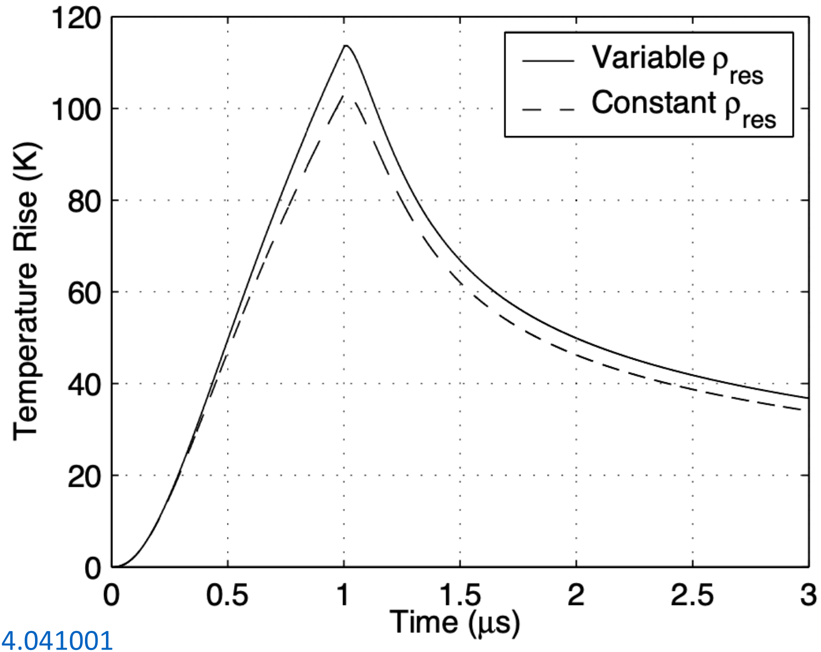
Pulsed Heating

- Without proper cooling temperature rise of ~100 K is expected

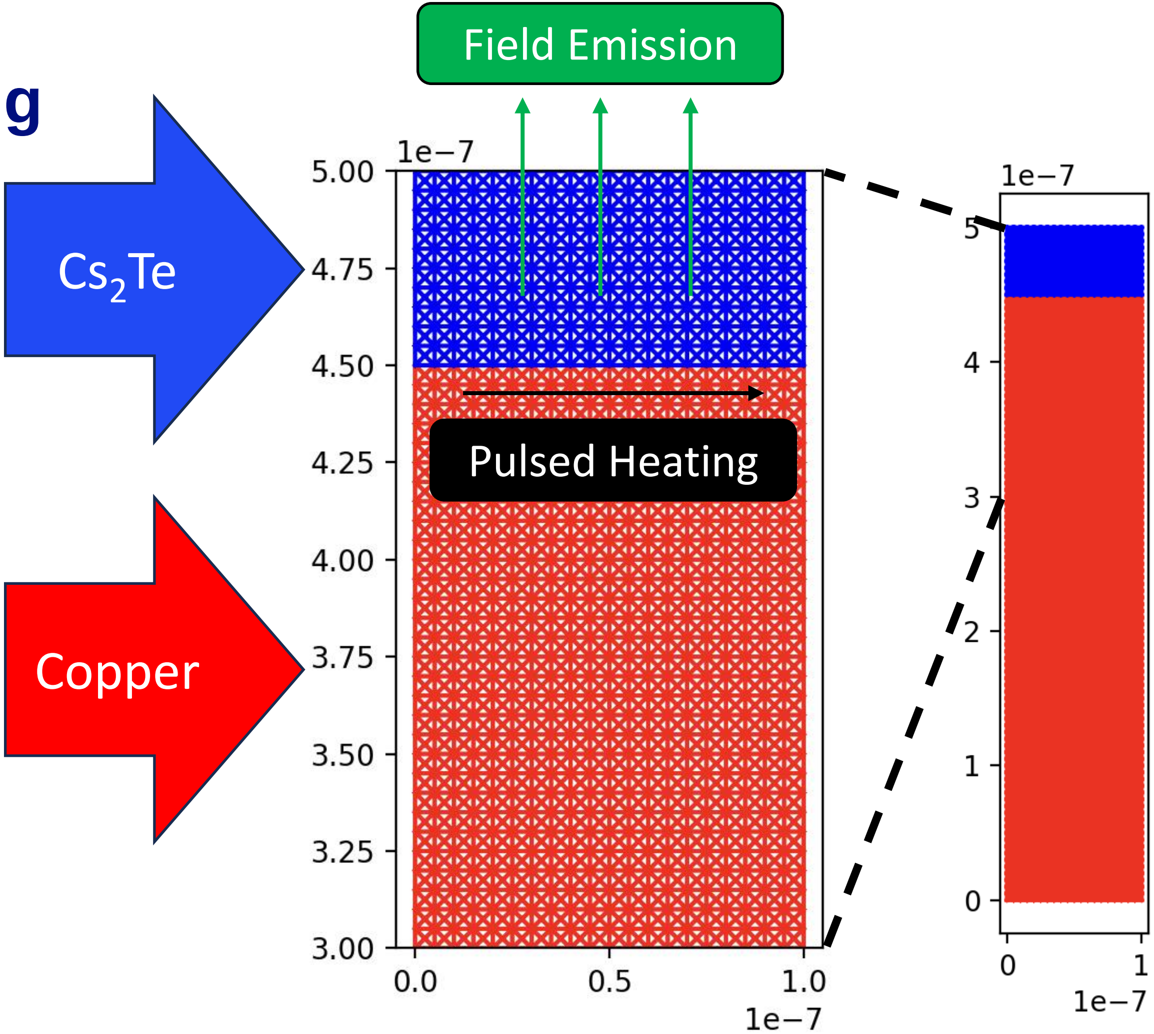


Lisa Laurent https://journals.aps.org/prab/abstract/10.1103/PhysRevSTAB.14.041001

David Pritzkau https://www.slac.stanford.edu/grp/arb/tn/arbvol3/ARDB271.pdf



Pulsed Heating



Acknowledgement

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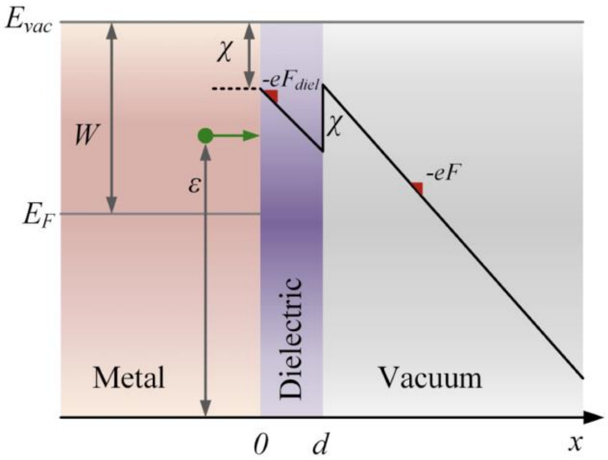
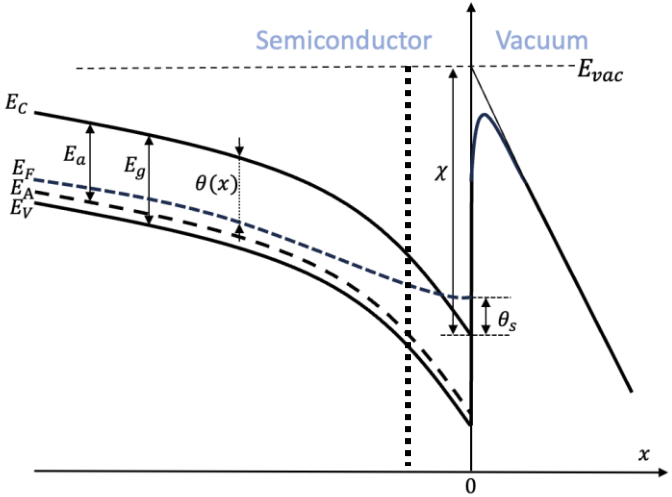
Assuming Double Triangle Energy Barrier

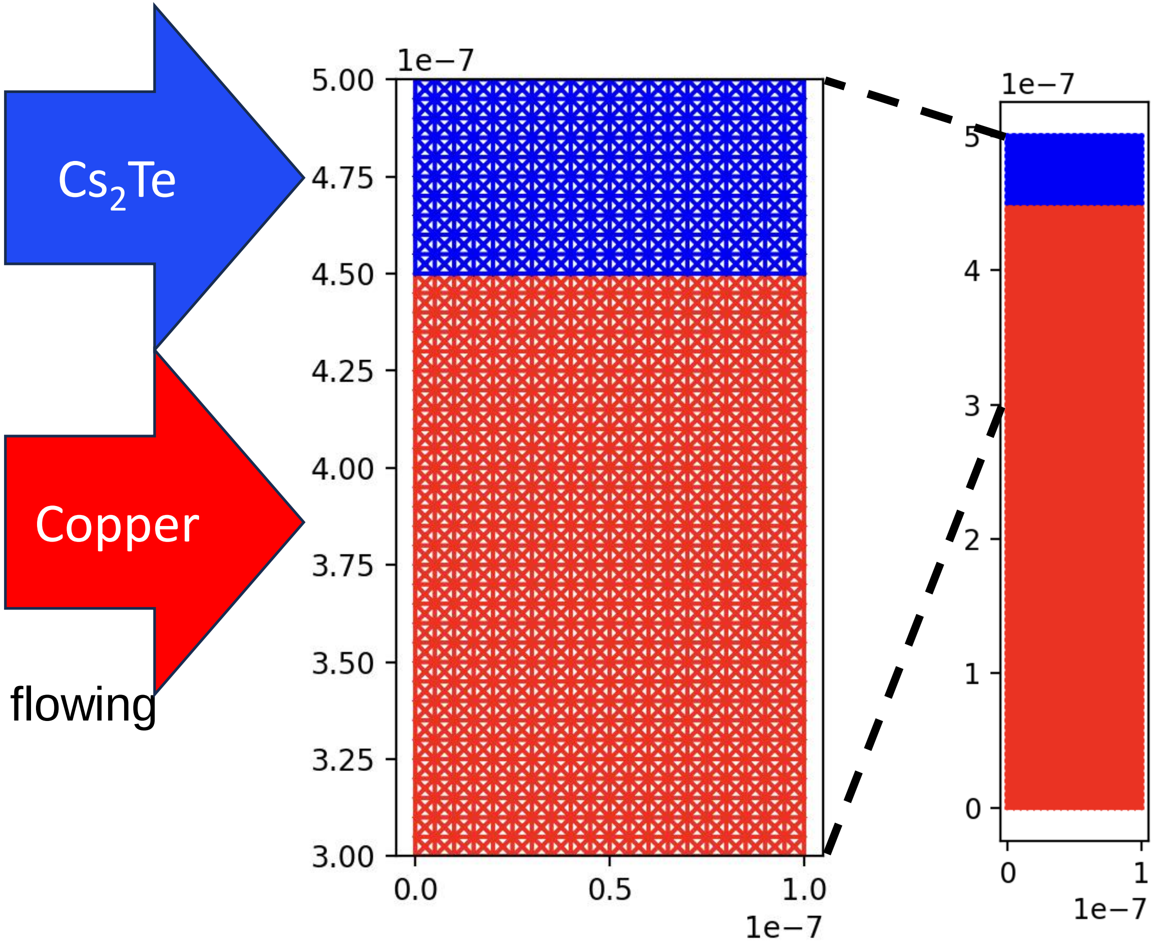
- Conduction-band near in the thin film follows the slope $-eF_{vacuum}$
- fermi level follows the slope $-eF_{diel}$
- linear relationship between Ec(x) and Ef(x) in the thin film





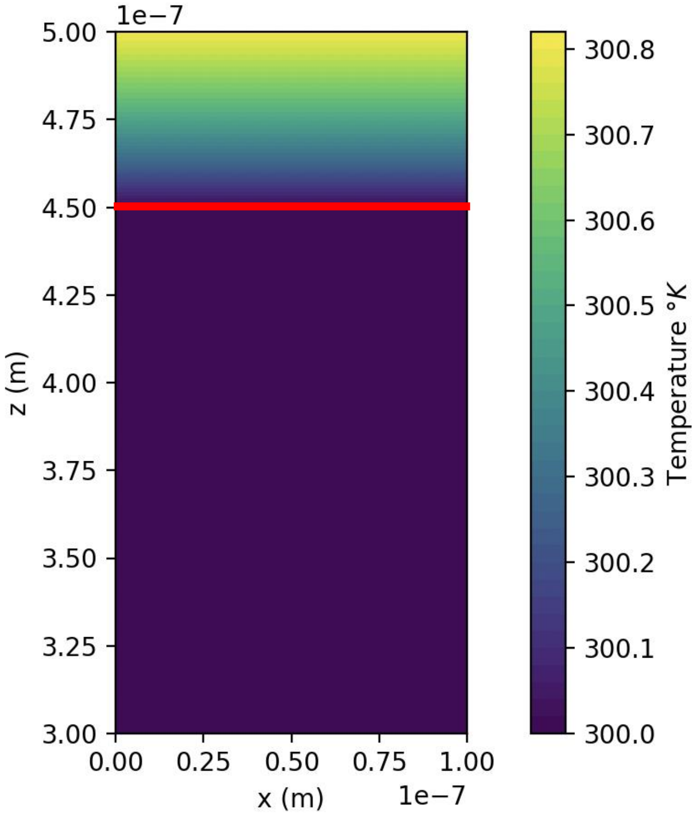
Simulation setup with copper layer

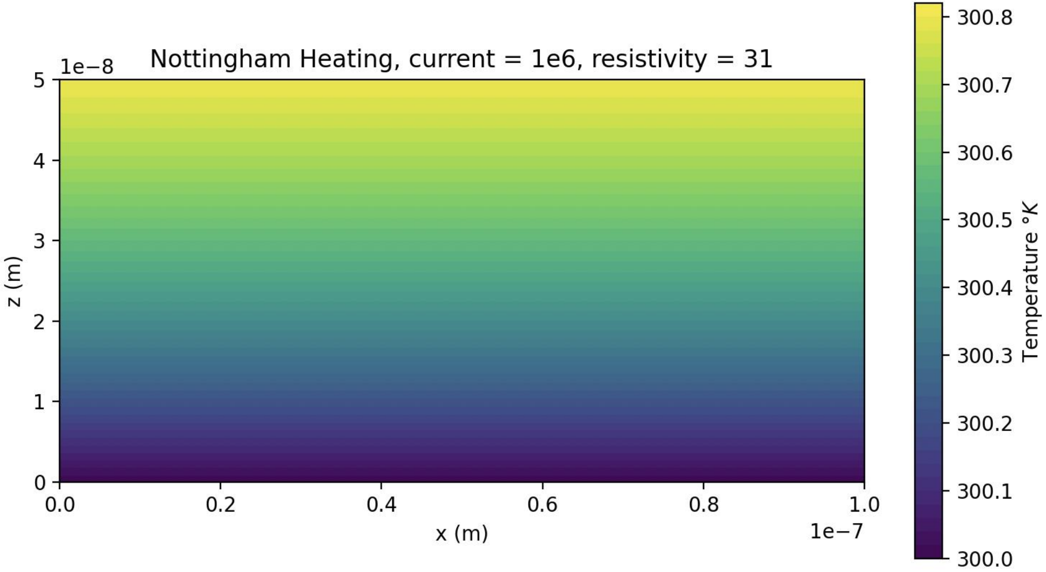
- 50 nm layer width
- Electrical Resistivity =
  - Cs2Te: 31 $\Omega \cdot m$
  - Copper: 1.68e-8 $\Omega \cdot m$
- Thermal Conductivity =
  - Cs2Te: 0.12 $\frac{W \cdot m}{\mathrm{K}}$
  - Copper: 386 $\frac{W \cdot m}{\mathrm{K}}$
- 1e6 A/m^2 current density flowing through Cs2Te



With Cs2te on top of copper layer

- Result is (basically) equivalent to boundary condition case ↓





Charge Density near surface

- $y(x) = \frac{E_F(x) - E_C(x)}{k * T/q}$
- Linear relation with x vs y
- Can calculate charge density near surface

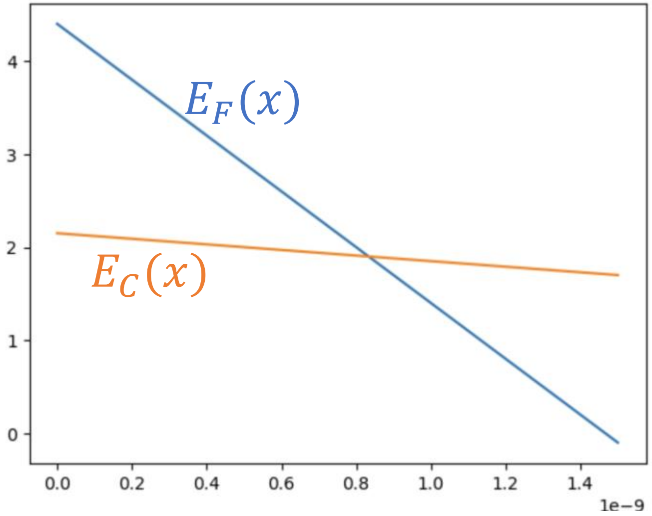
$$n(y) = N_C F_{1/2}(y),$$

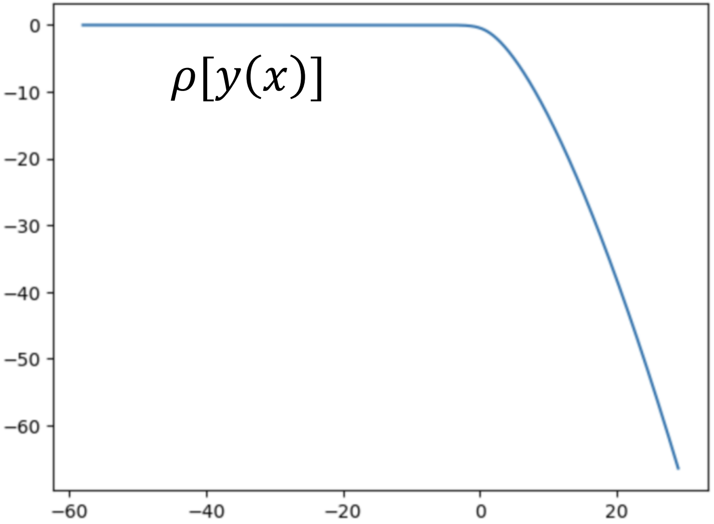
$$p(y) = N_V F_{1/2}(-E_g/k_B T - y),$$

$$N_a^-(y) = \frac{N_a}{1 + 2\exp\left(-E_a/k_B T - y\right)},$$

$$N_d^+(y) = \frac{N_d}{1 + 2\exp\left(E_d/k_B T + y\right)}.$$

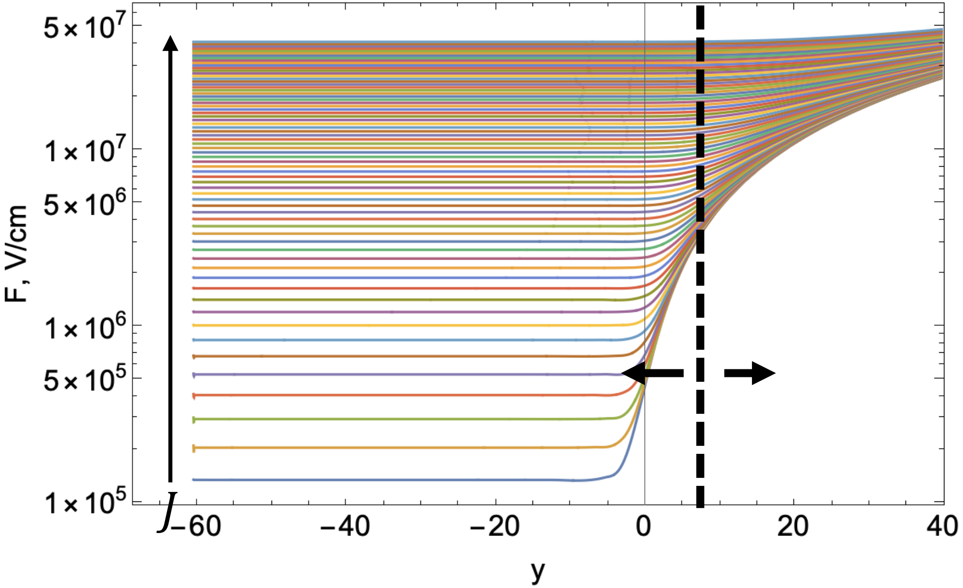
$$\rho = -q(n - p + N_a^- - N_d^+).$$





Result

- Each colored line represents a different current.
- Surface field/current can be determined by the assumed y (surface)



Current vs Field Preliminary Result