Computational modeling of RF breakdown precursor formation on accelerator surfaces

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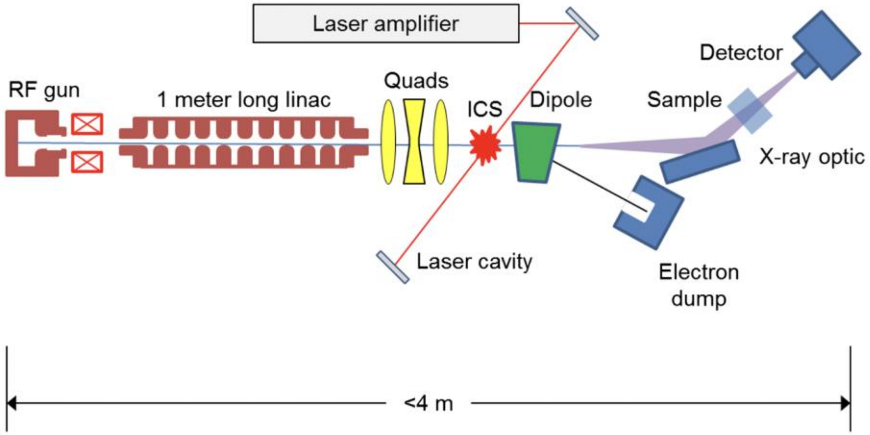
Table of Content

Introduction – Next Generation High Gradient Application

- Future Electron/light source
  - Miniaturization (C-, X-band)
  - High applied field/gradient
- Normal Conducting HG Application
  - Travelling wave linear accelerator (CLIC)
  - Photoinjectors: SLAC (X-band), LANL (C-band)
  - Free Electron Laser
  - Compact light sources
  - Etc.
- Application of high-field gradient (>100 MV/m)



Introduction – Next Generation High Gradient Application

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  - Etc.
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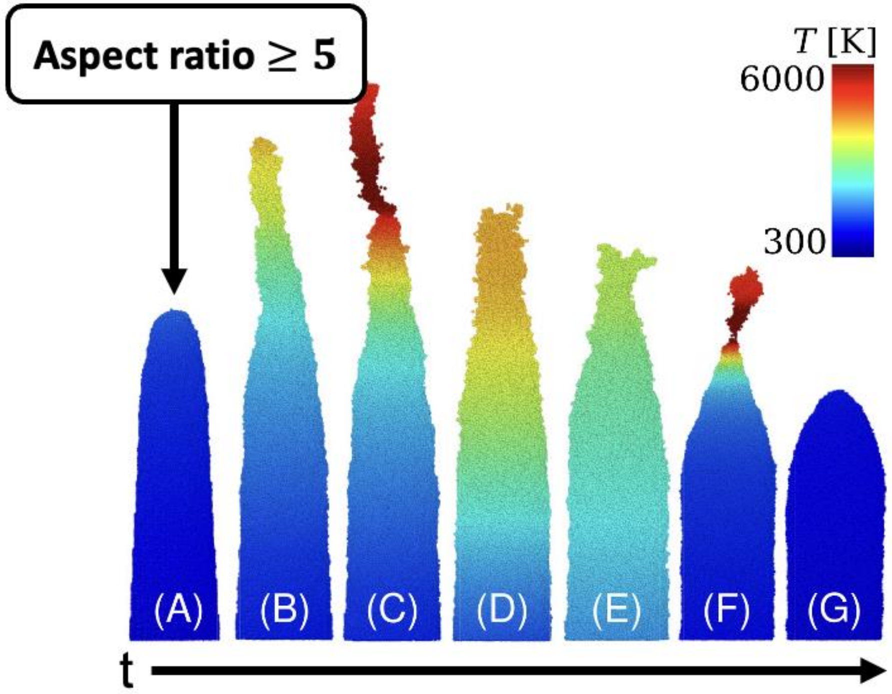
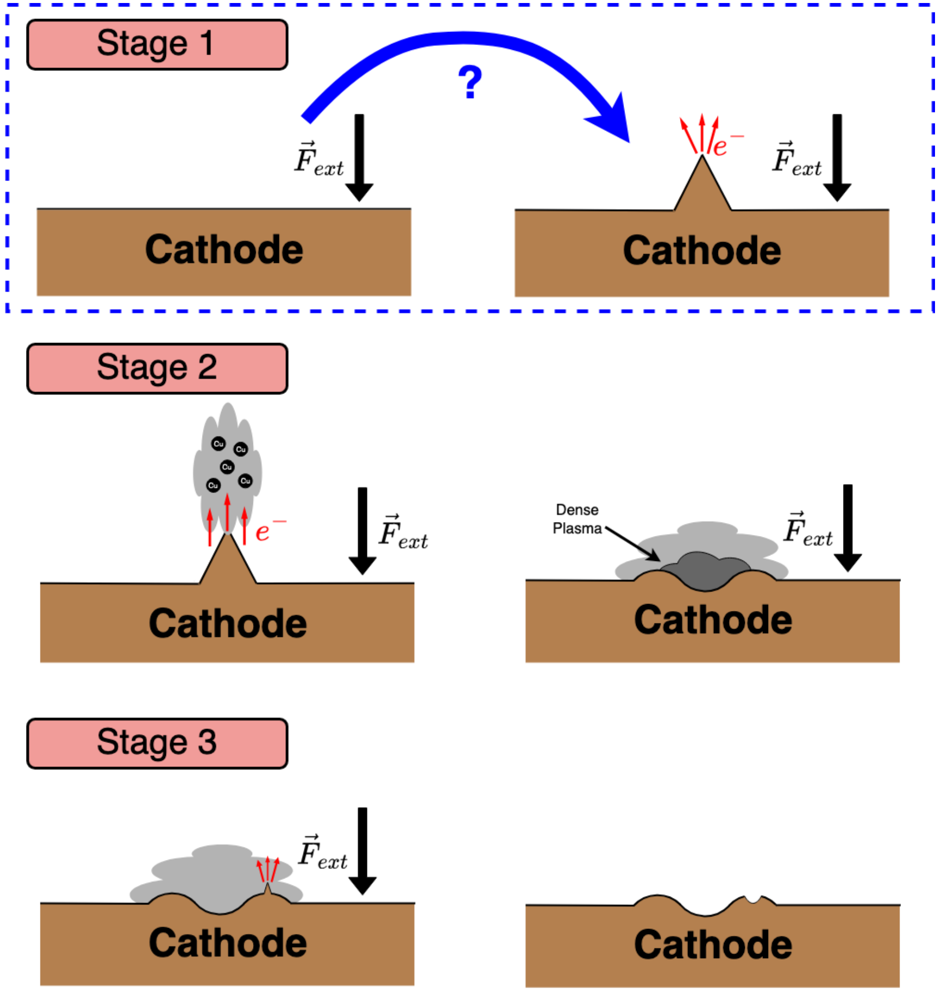
RF Breakdown

Breakdown Nucleation Process

Breakdown nucleates from sharp emitter

- Recent computational models shows that thermal runaway process could melt metals to the vacuum





Thermal runaway of metal nano-tips during intense electron emission

A Kyritsakis, M Veske, K Eimre, V Zadin and F Djurabekova

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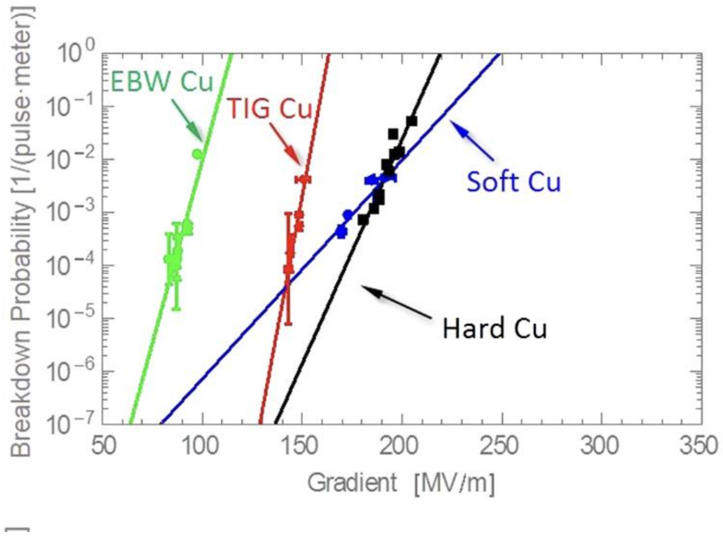
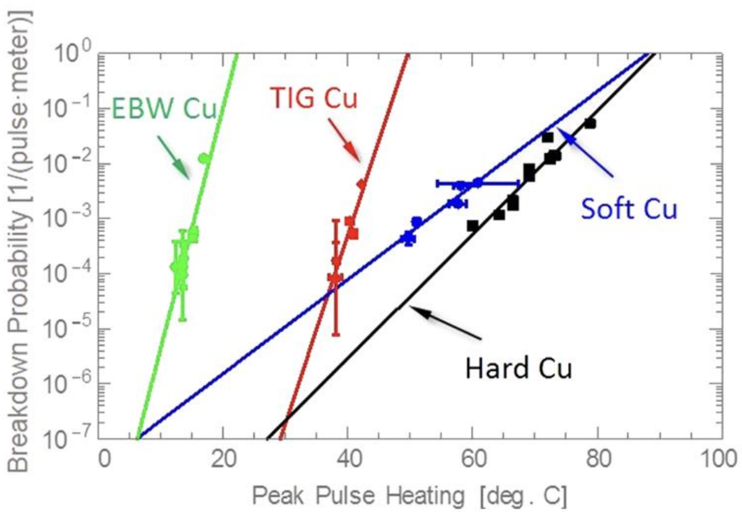
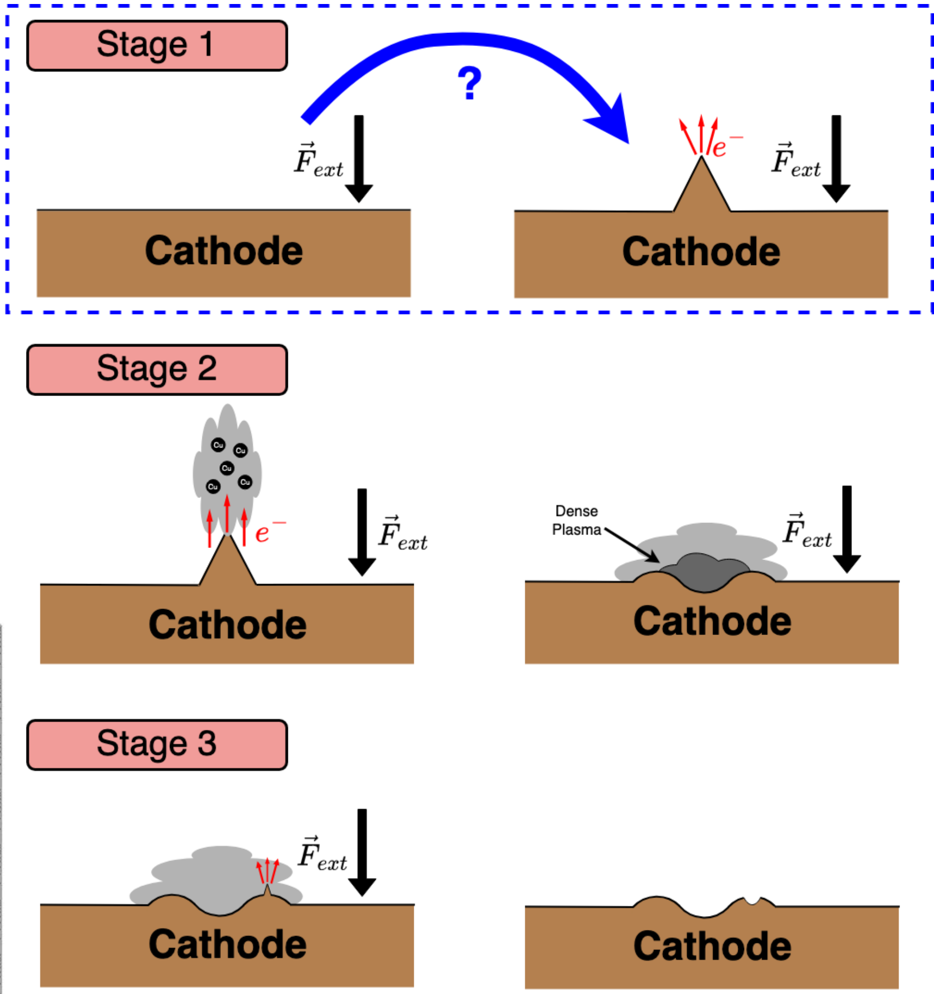
Breakdown Precursor Formation

- Motivation
  - Unveil the **formation mechanisms** of **precursors** that can lead to breakdown
- Interested in two parameters
  - Field Gradient/Pulsed heating

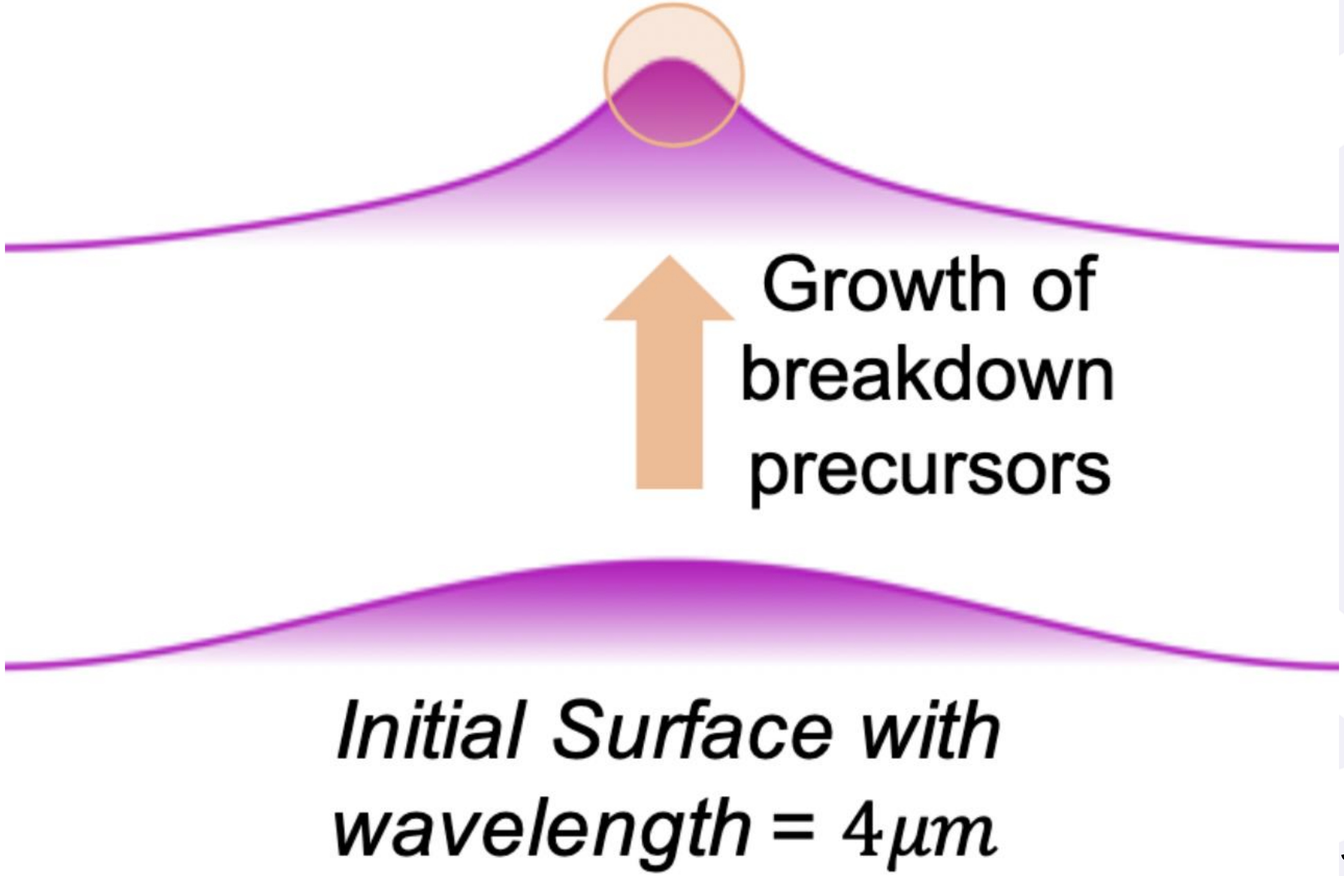






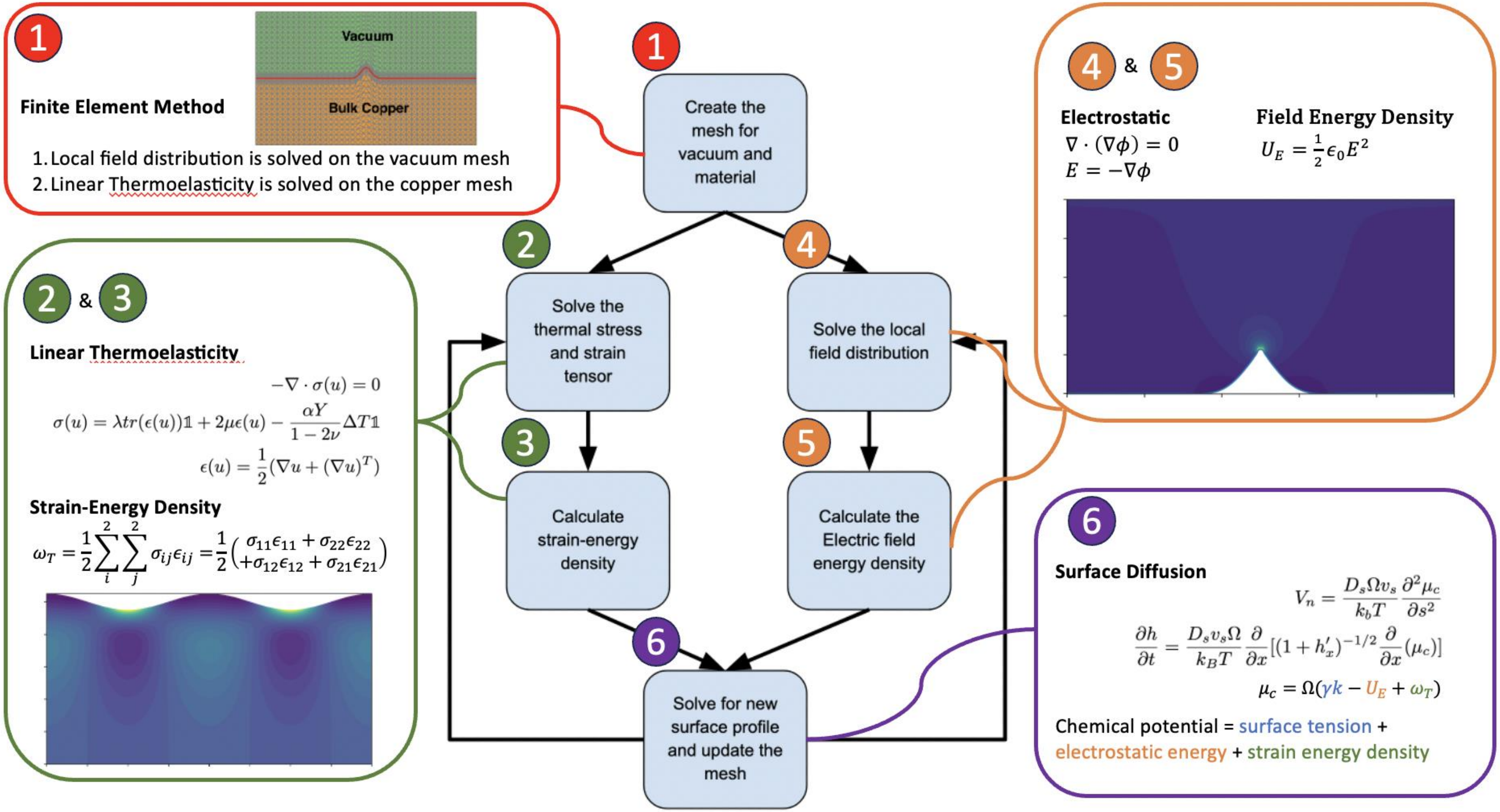
Breakdown Precursor Formation: surface diffusion

- Computational model: Breakdown precursor formation from low amplitude surface



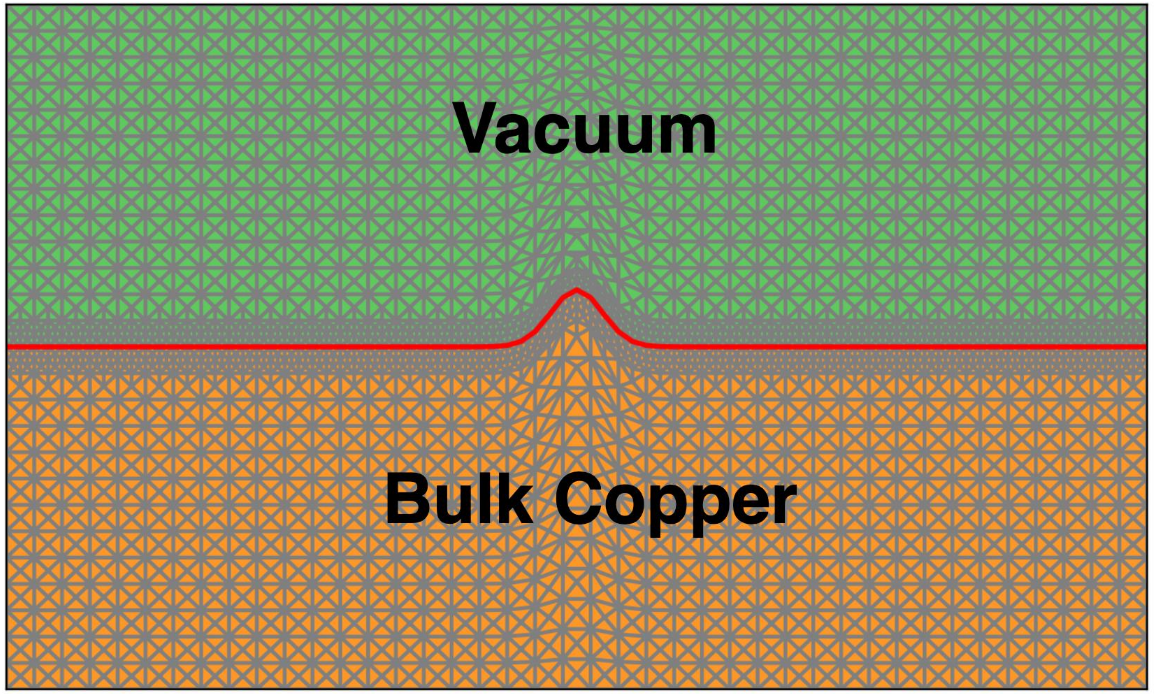
Soumendu Bagchi (2018)

Curvature Driven Surface Diffusion Model Flow Chart



Problem Formulation 1

- Consider 2 input parameter
  1. Applied Field
  2. Pulsed Heating
- Finite Element Method
  - 2D domains for the **vacuum** and bulk **copper** material
  - Local field distribution is solved on the vacuum mesh
  - Linear Thermoelasticity is solved on the copper mesh



Linear Thermo-elasticity 2 & 3

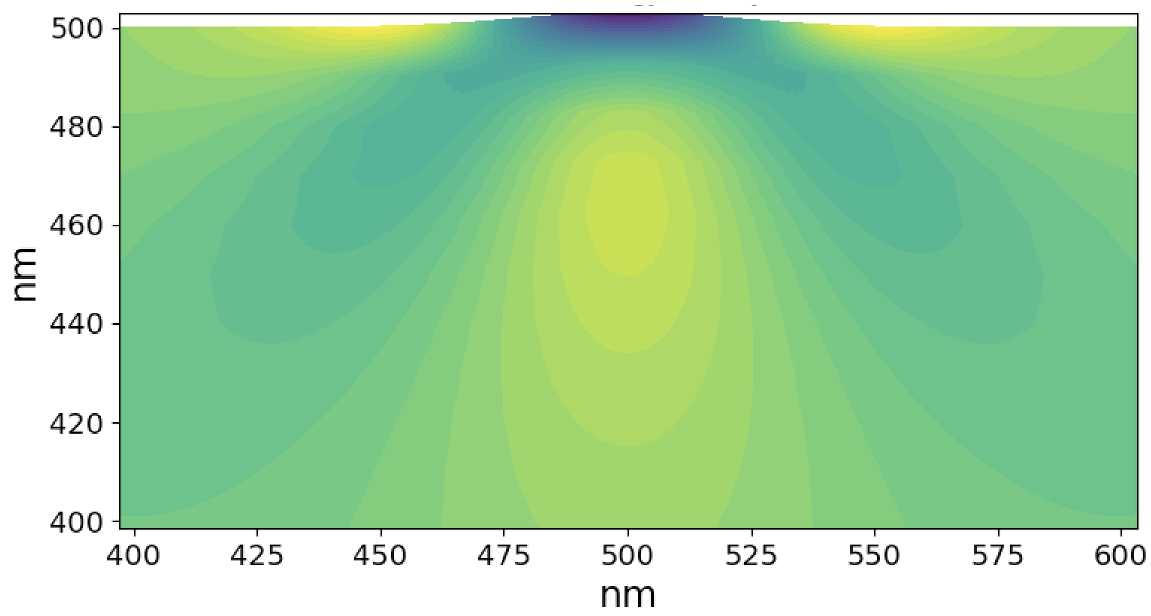
- u = deformation vector
- $\sigma(u)$ = stress tensor
- $\epsilon(u)$ = infinitesimal strain te

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

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

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

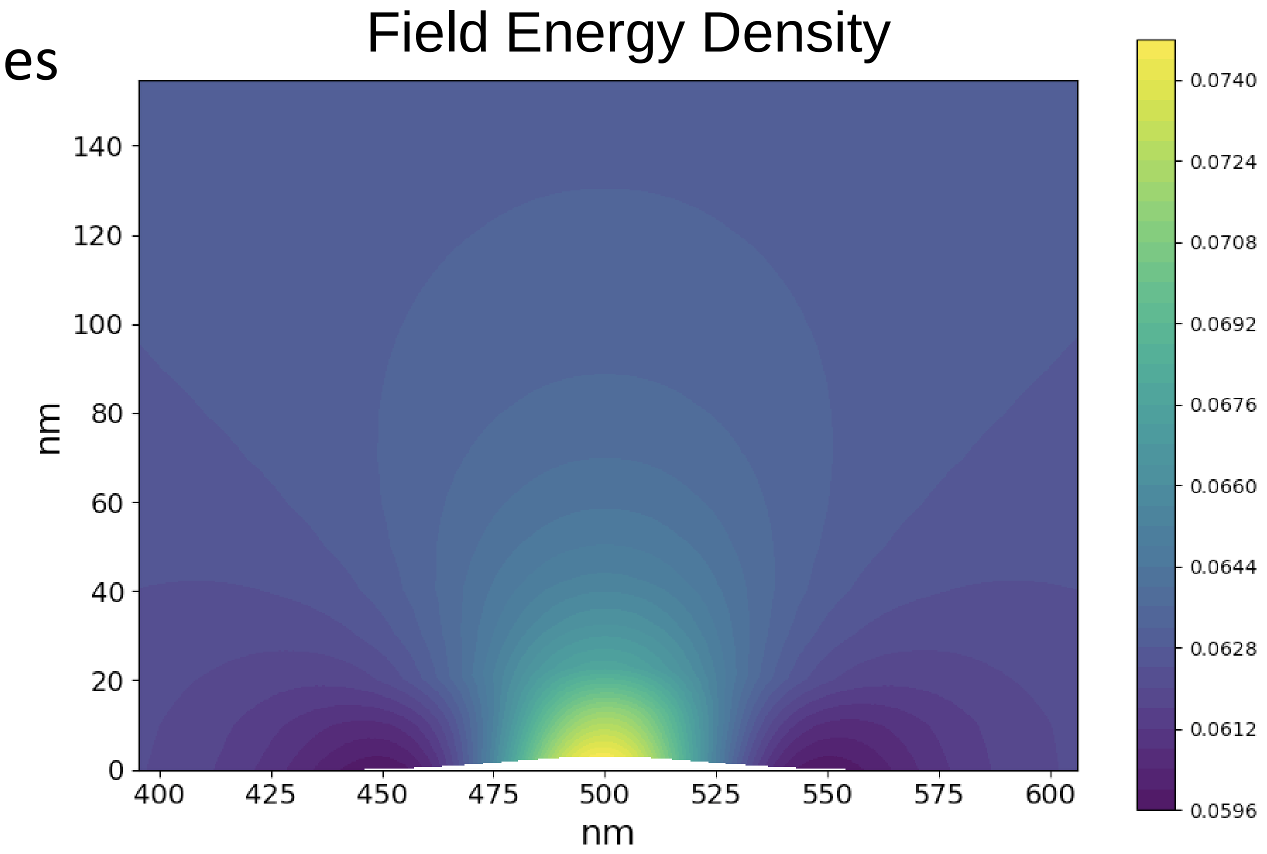
Strain Energy density



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

Field Energy Density 4 & 5

- **Formulation**
  - Governing Equation and boundary values
    - $-\nabla^2 \varphi = 0$ in vacuum
    - $\varphi = 0$ on material surface
    - $-\nabla \varphi \cdot \vec{n} = E_h$ as applied field
  - The energy density on the material surface is
    - $E = -\nabla \varphi$
    - $\boldsymbol{U = \frac{1}{2} \epsilon_0 E^2}$



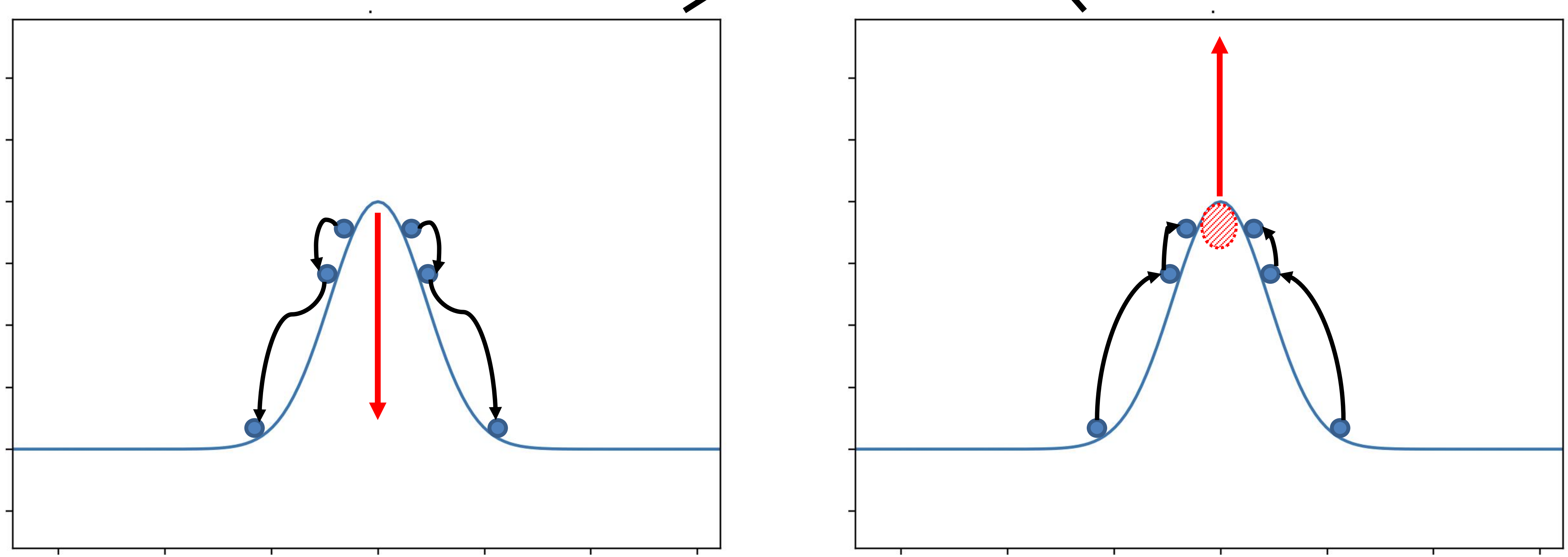
Surface Diffusion Formulation 6

Diffusion Flux

$$J = -\frac{D_s}{kT}\left(\frac{\partial \mu}{\partial s}\right), \mu = \gamma\kappa + \omega_{EM}$$

Surface Tension

E-M Energy



Surface Diffusion Formulation

Normal Velocity

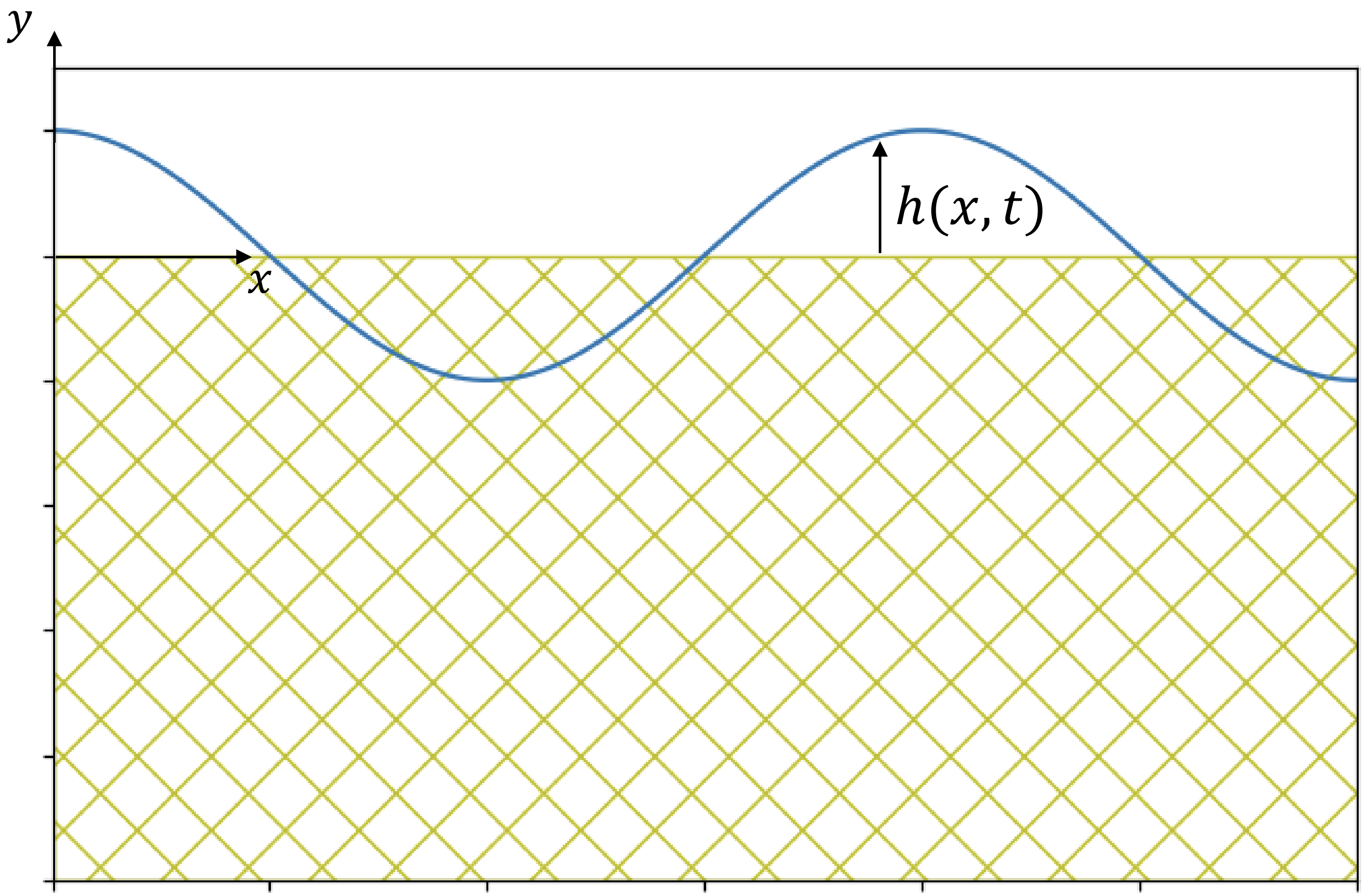
- $\nabla \cdot J \rightarrow$ change in # of atom per unit area per unit time

$$V_n \propto \nabla \cdot J \qquad (2)$$

$$V_n = \frac{D_s \Omega^2 \nu_s}{kT} \left(\frac{\partial^2 (\gamma\kappa + \omega)}{\partial s^2} \right)$$

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{t}} = \frac{\partial}{\partial \boldsymbol{s}} \left[\frac{\partial}{\partial \boldsymbol{x}} (\boldsymbol{\gamma\kappa} + \boldsymbol{\omega}) \right] \qquad (3)$$

Governing Equation



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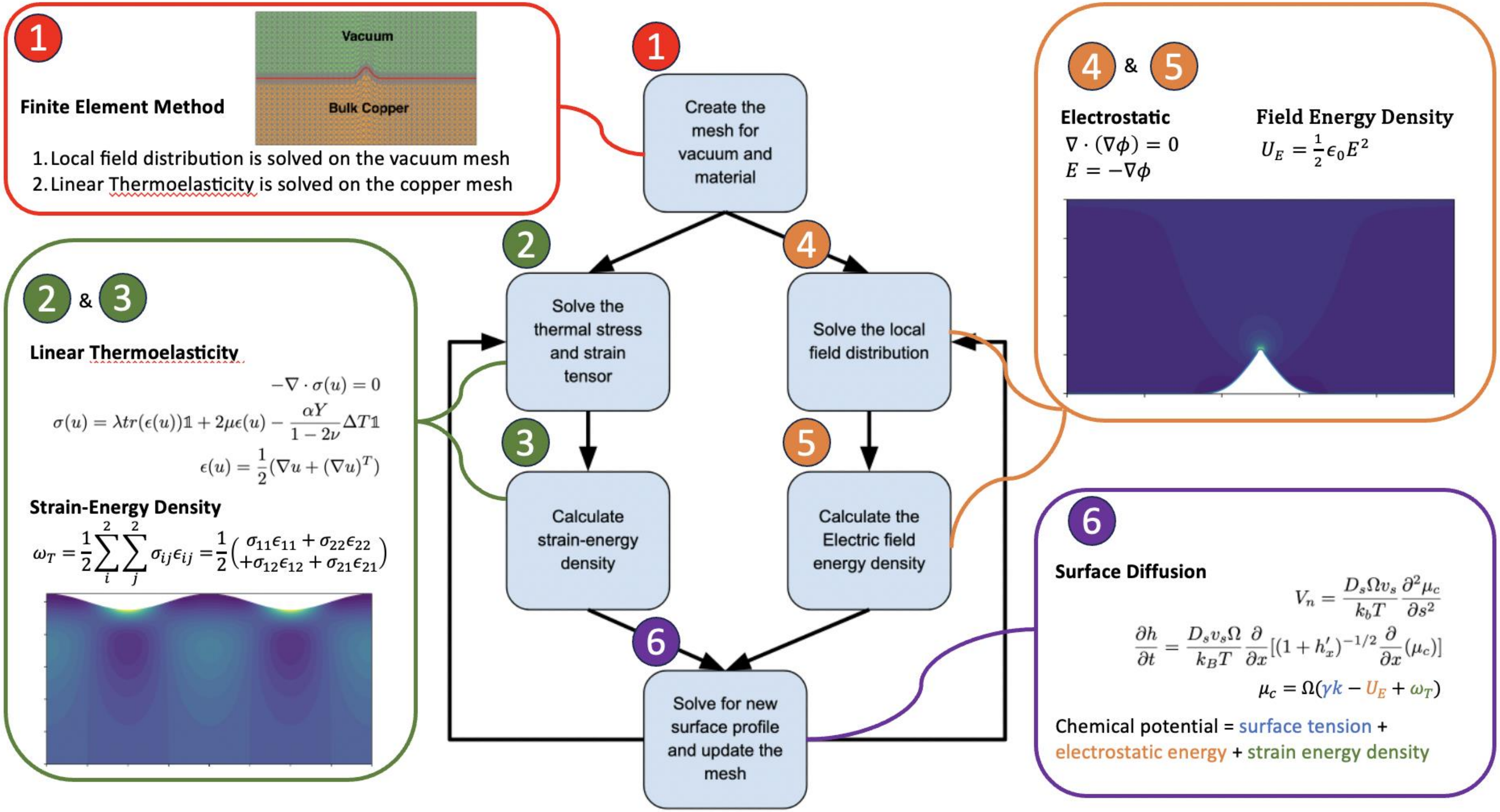


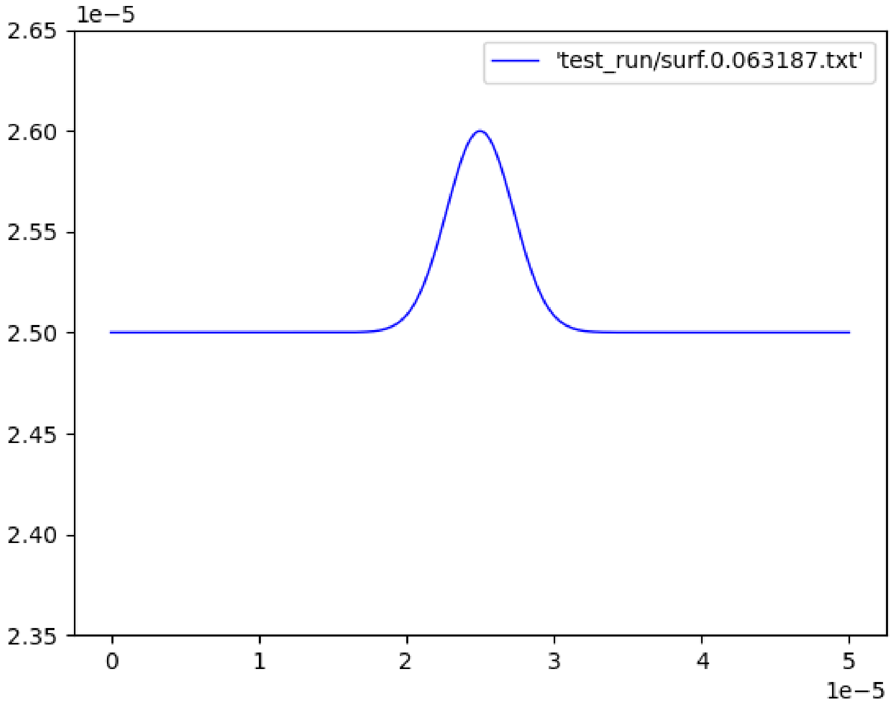
Computational Method

- Finite Element Method
- Utilize Open-source project called **FEniCS**
  - Provide scientific computing tools for working with computational meshes, finite-element variational formulations of ordinary and partial differential equations
  - variational forms are specified in the high-level Python-based Unified Form Language (UFL)
  - executed through high-performance computational kernels using the finite element library DOLFIN

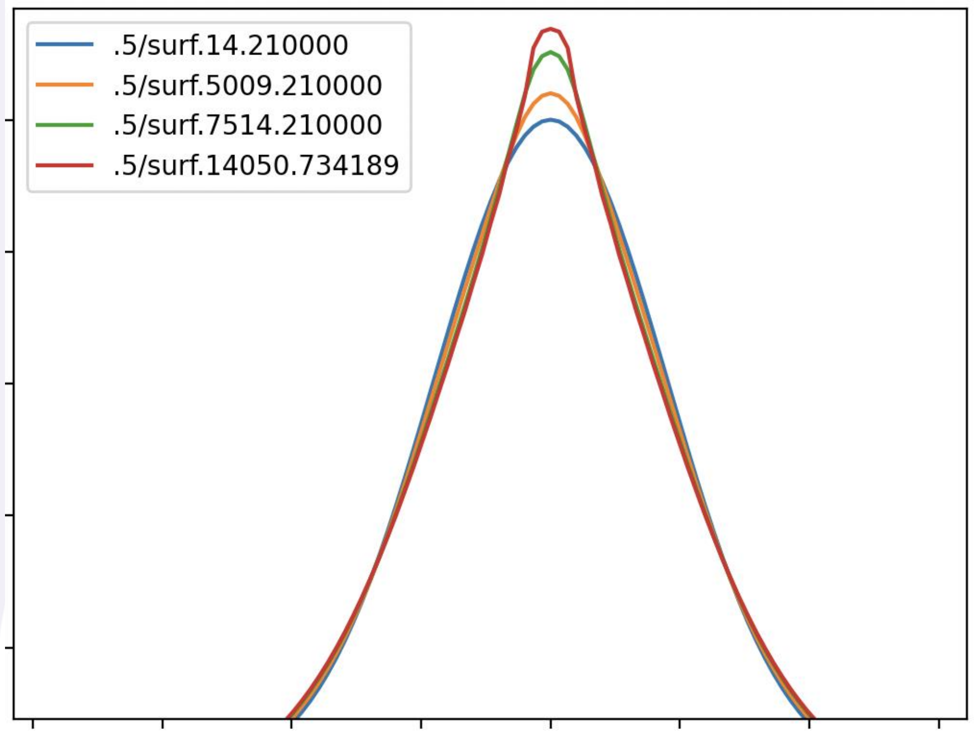
Result

Field/Heating surface evolution mechanism

- **Heating**
  - Dominated by grooving
  - **Secondary groove/peak formation due to surface transport and volumetric conservation**

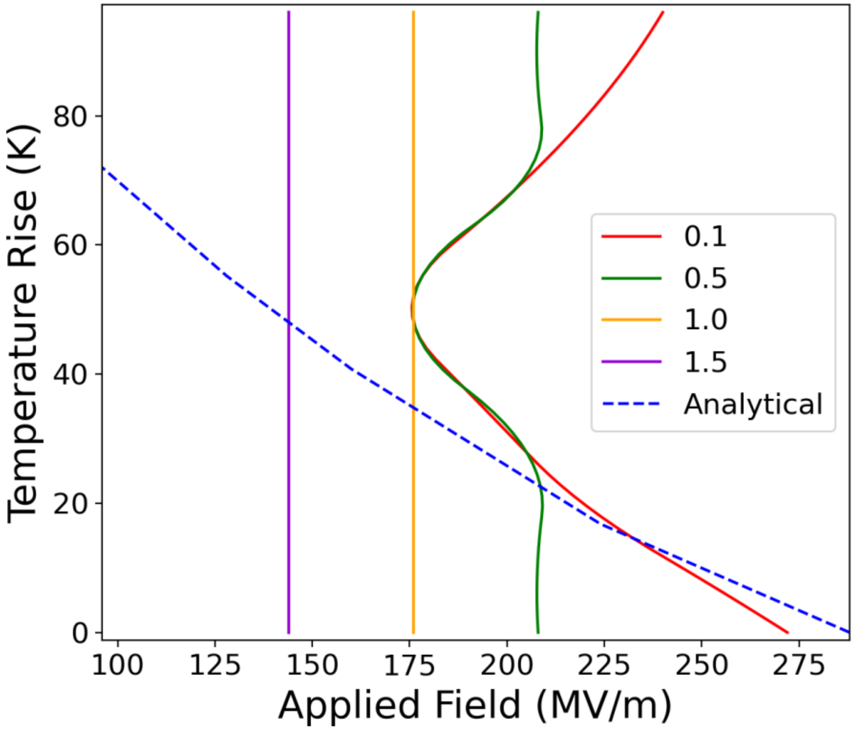


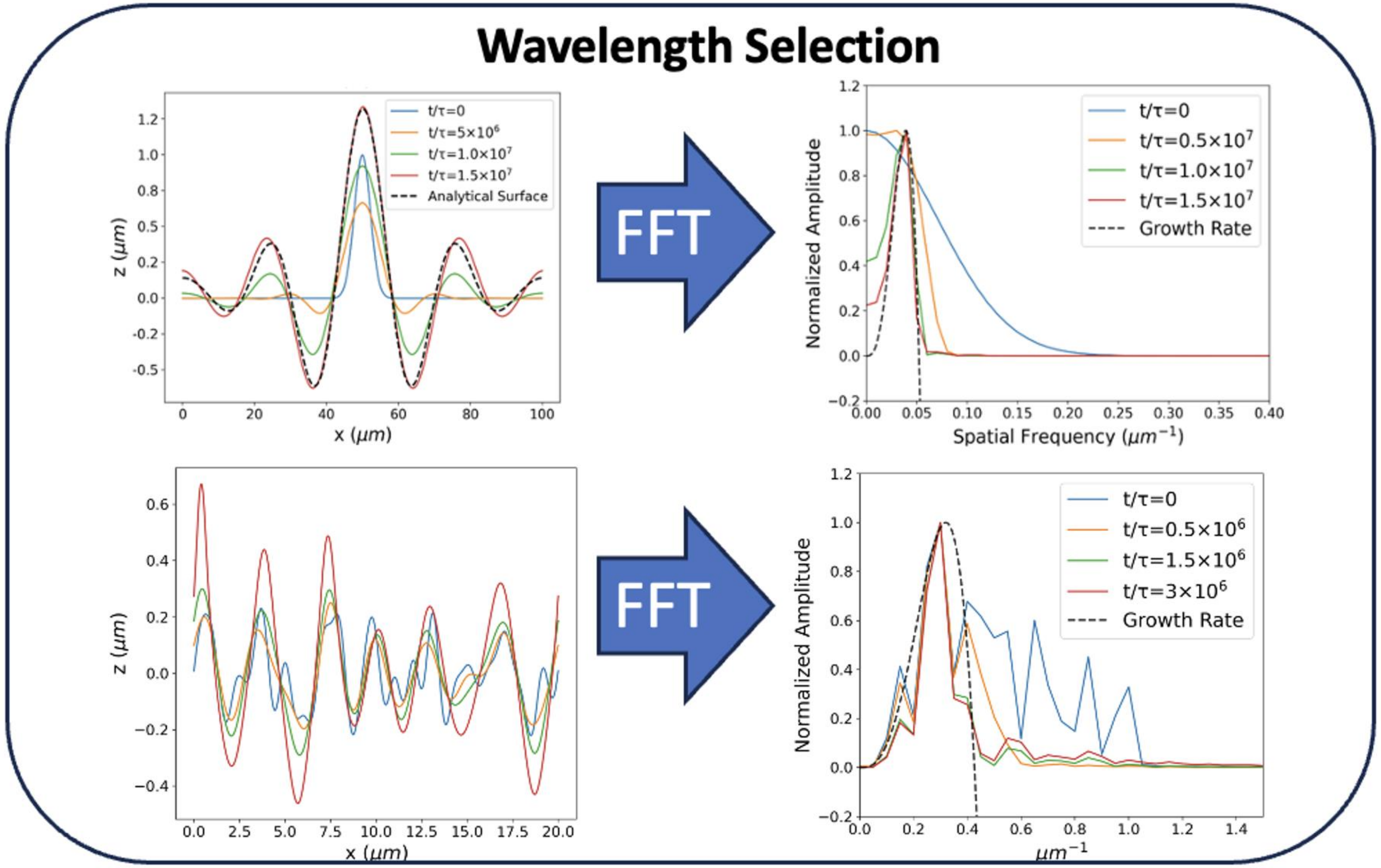
- **Field**
  - Create a sharp tip



Combined Effect

- Surface diffusion allows synergistic effect to take place
  - Surface Reorganization
  - Wave-length selection



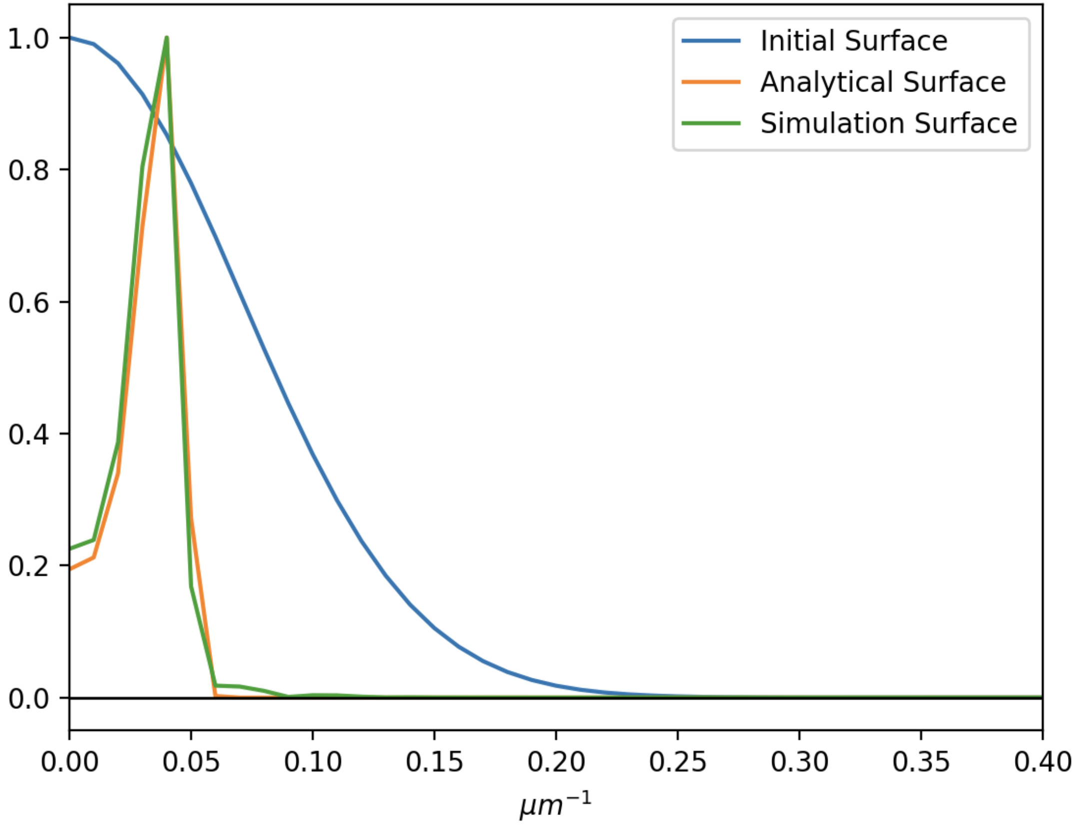


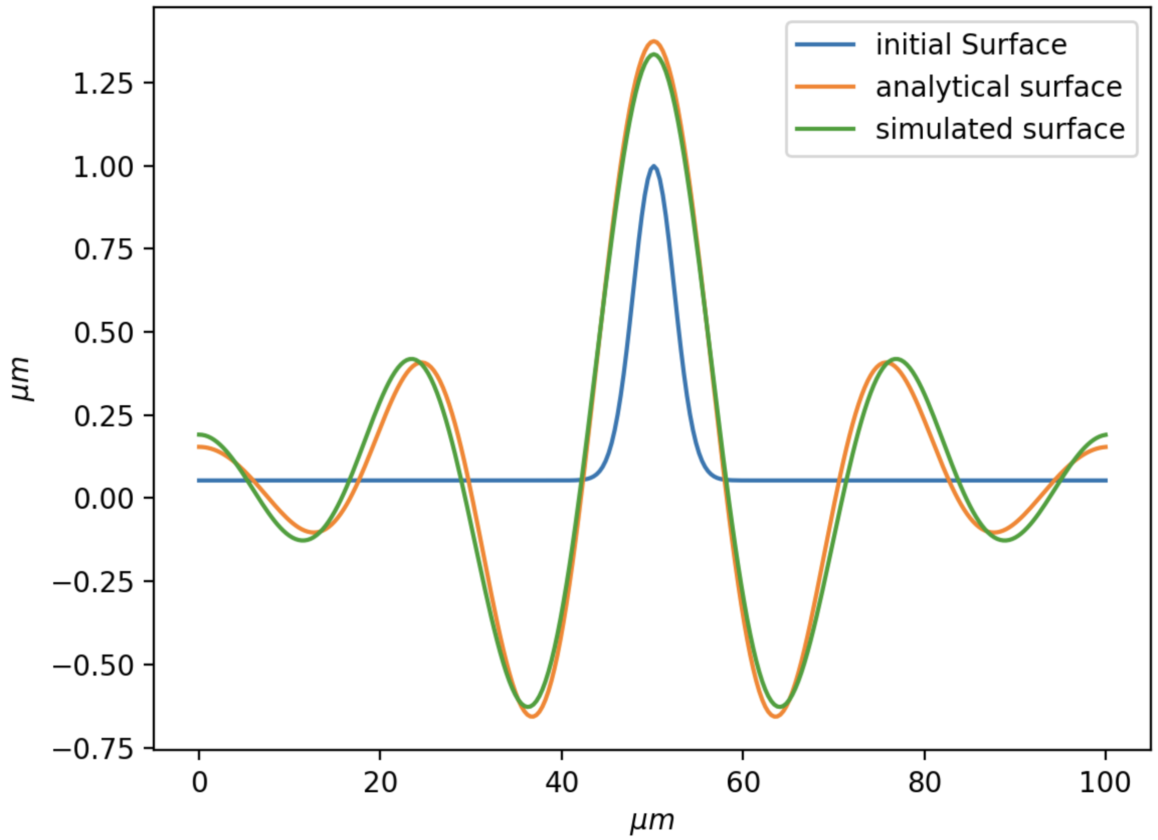
Systematic Analysis of Surface Morphology

- Linear Stability Analysis (small amplitude approximation)
  - Small amplitude approximation A*k sin(k x)
  - Solving $\frac{\partial h}{\partial t} = C\frac{\partial^2 \mu}{\partial x^2}$
  - Solution in the frequency domain takes the form
    - $h(t, k) = h_0 \exp(g(k) * t)$
    - Where $g(k)$ is the growth rate
- $h(t, k) = \mathrm{h}_0(k)\exp(C\left(2k^3\alpha^2\boldsymbol{\Delta T^2} + k^3\epsilon_0\boldsymbol{E^2} - \gamma k^4\right)t)$

Agreement with small amplitude approximation

- Given Initial gaussian surface -> take FFT of the surface and multiply it by
- $h(t,k) = \mathrm{h}_0(k)\exp(C\left(2k^3\alpha^2\boldsymbol{\Delta T^2} + k^3\epsilon_0\boldsymbol{E^2} - \gamma k^4\right)t)$





Random Surface Simulation

Surface: Modeled from surface scan of copper photocathode

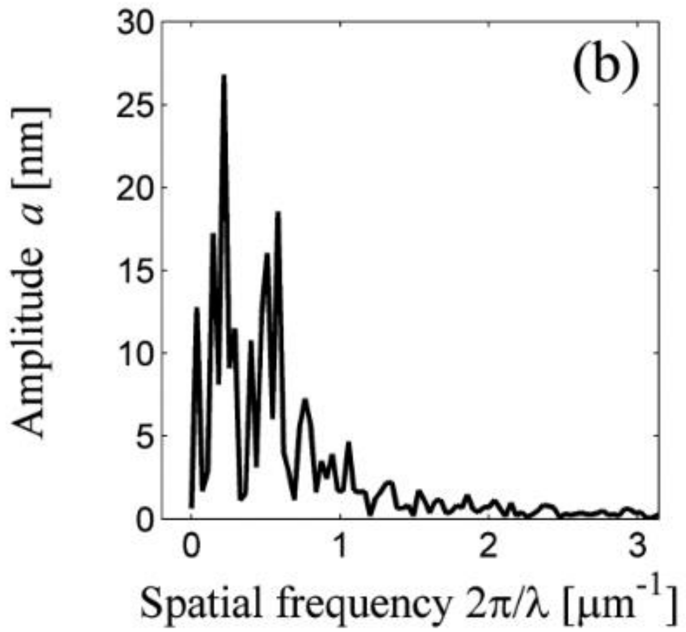
$$h(x) = \sum_{n}^{N} A_n sin(n\omega x + \phi_n)$$

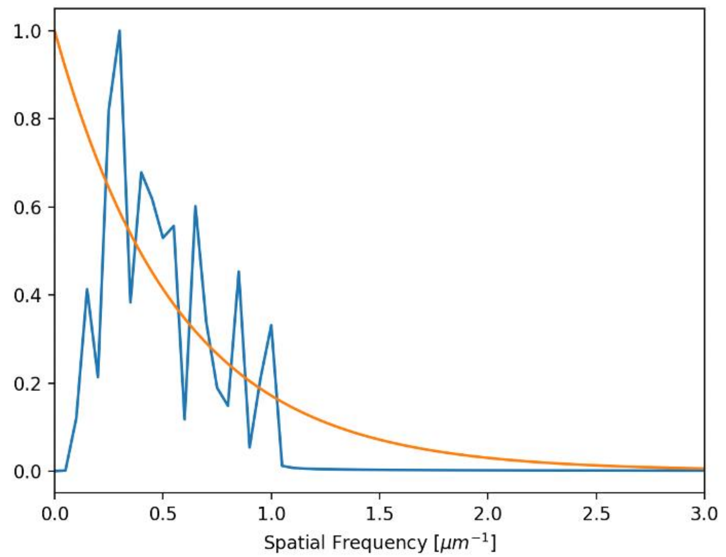
Parameters:

$$E_{applied} = 400MV/m$$

$$\Delta T_{applied} = 170K$$

$$\frac{2\pi}{k_m} = \lambda_m = 3.125\,\mu m$$





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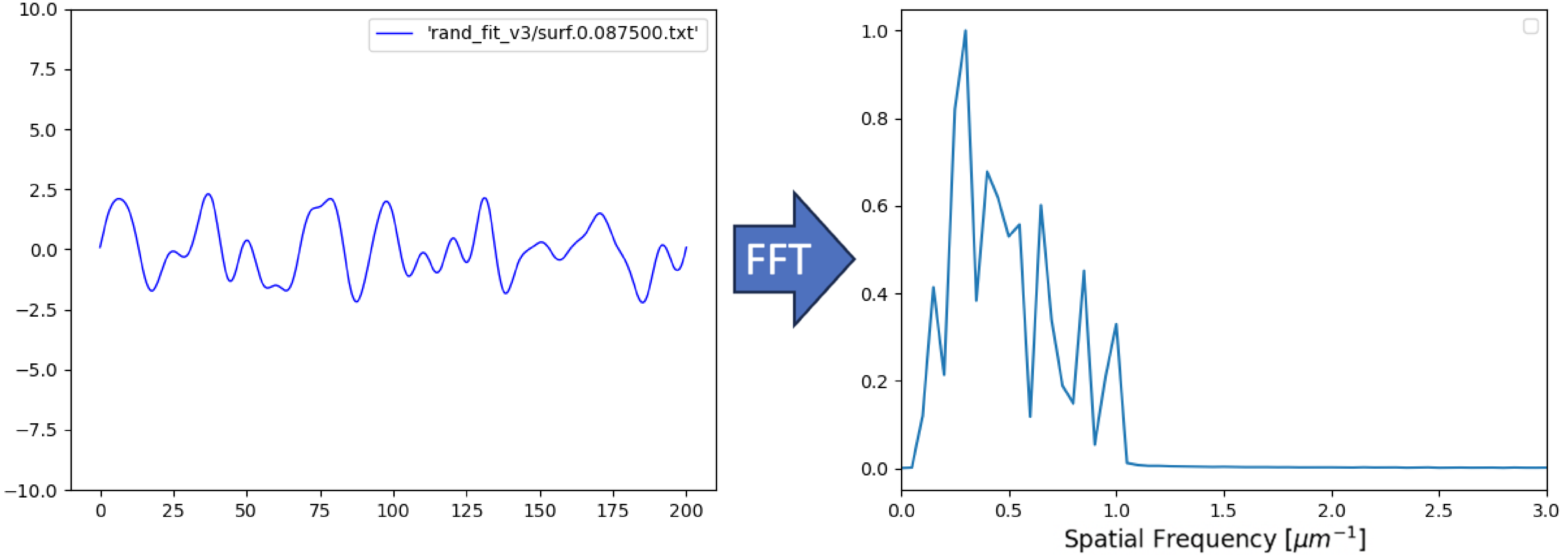
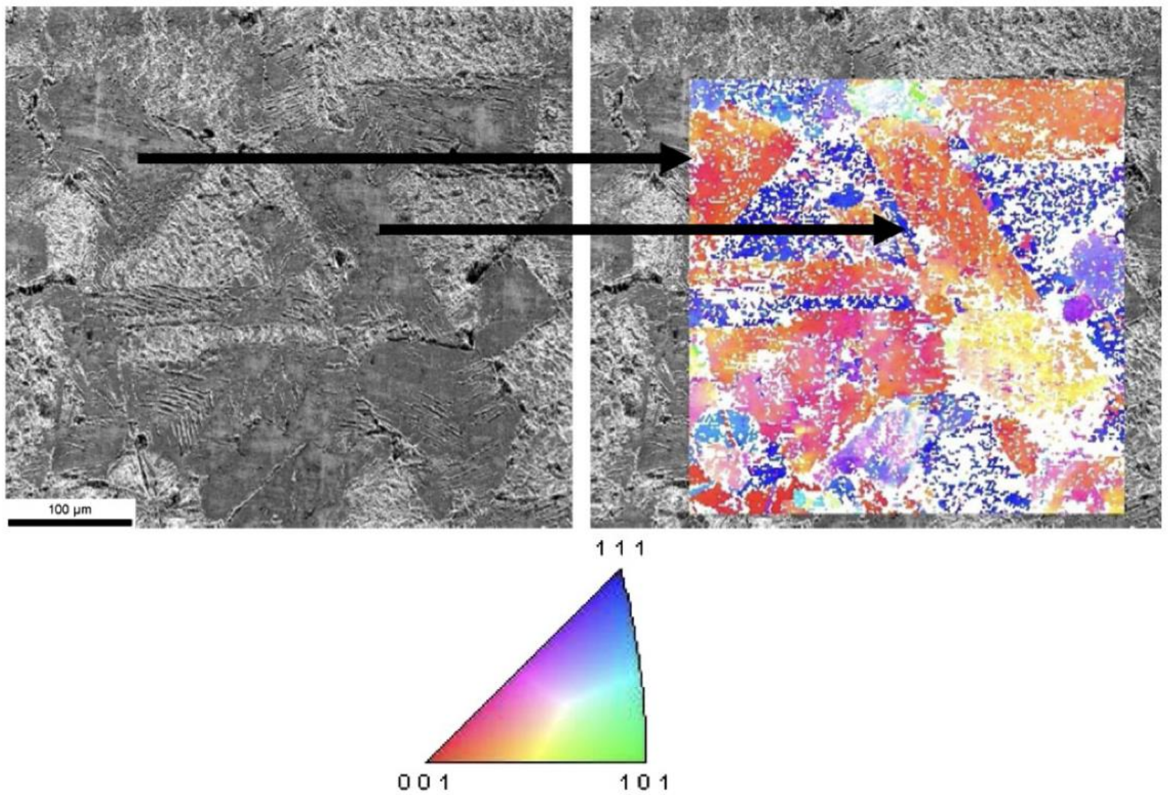


Roughness Development

- Diffusion Time-scale heavily reliant on **migration energy barrier**
  - $D_s \propto exp(-E_b/k_bT)$
- Experimental agreement with pulsed heating roughness development
  - They saw roughness development
  - (111)>(110)>(100)
  - While E_b follows: (111)<(110)<(100)

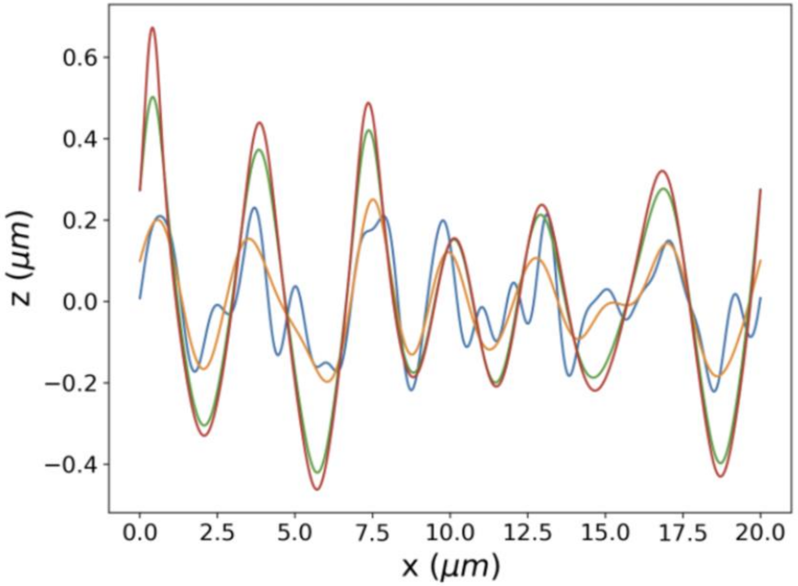
Experimental study of rf pulsed heating

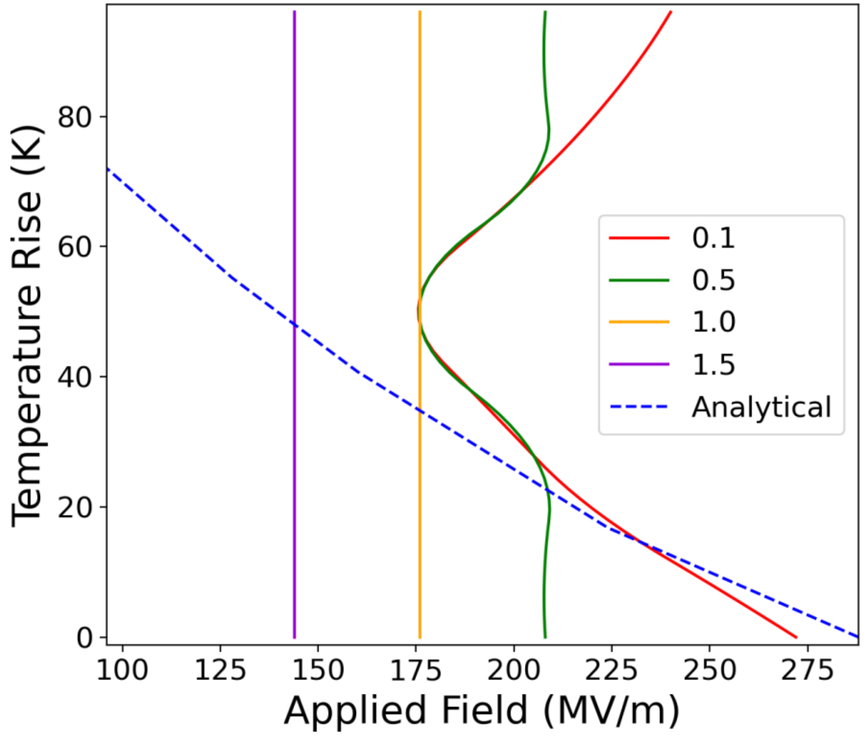
Lisa Laurent,* Sami Tantawi, Valery Dolgashev, and Christopher Nantista
SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA



Conclusion

- RF Pulsed heating and E-Field works in tandem to create a sharp emitter like geometry through surface reorganization
- Comparative experimentally expected values
  - $\Delta T \approx 60$ K
  - $E_{surface} \approx 150 - 200$ MV/m
  - Initial surface aspect ratio (height/width) = 0.1





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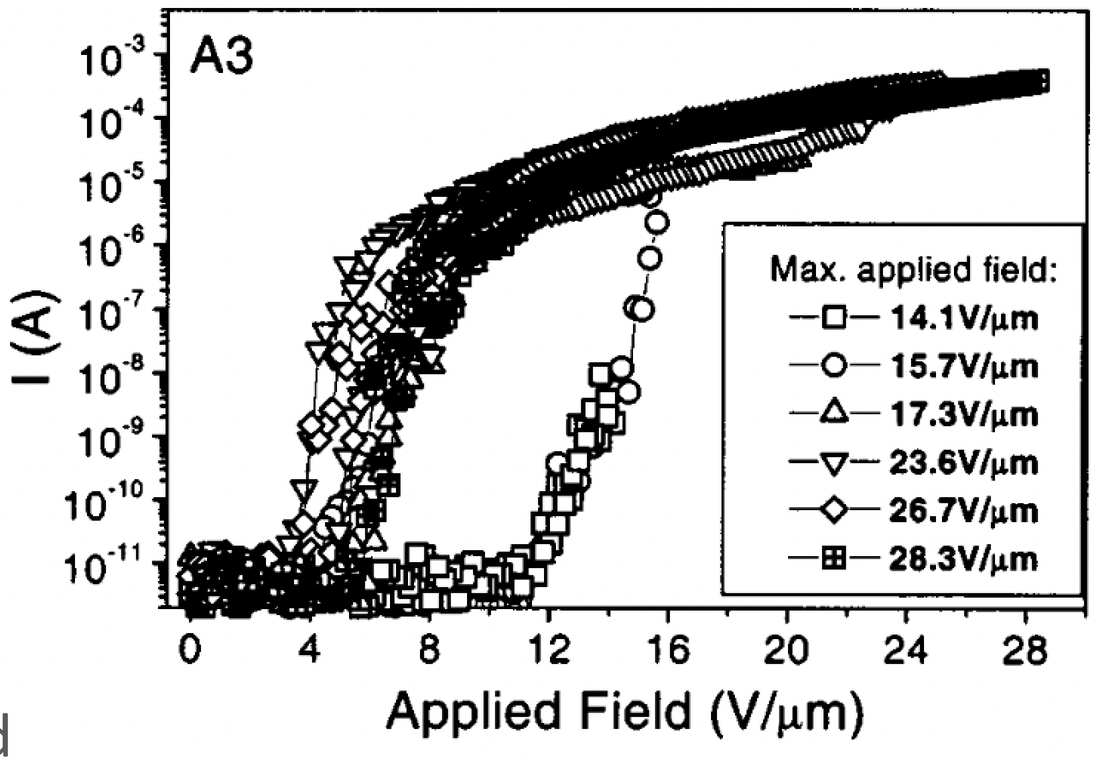
Semiconductor Current profile

Deviation from classical FN equation

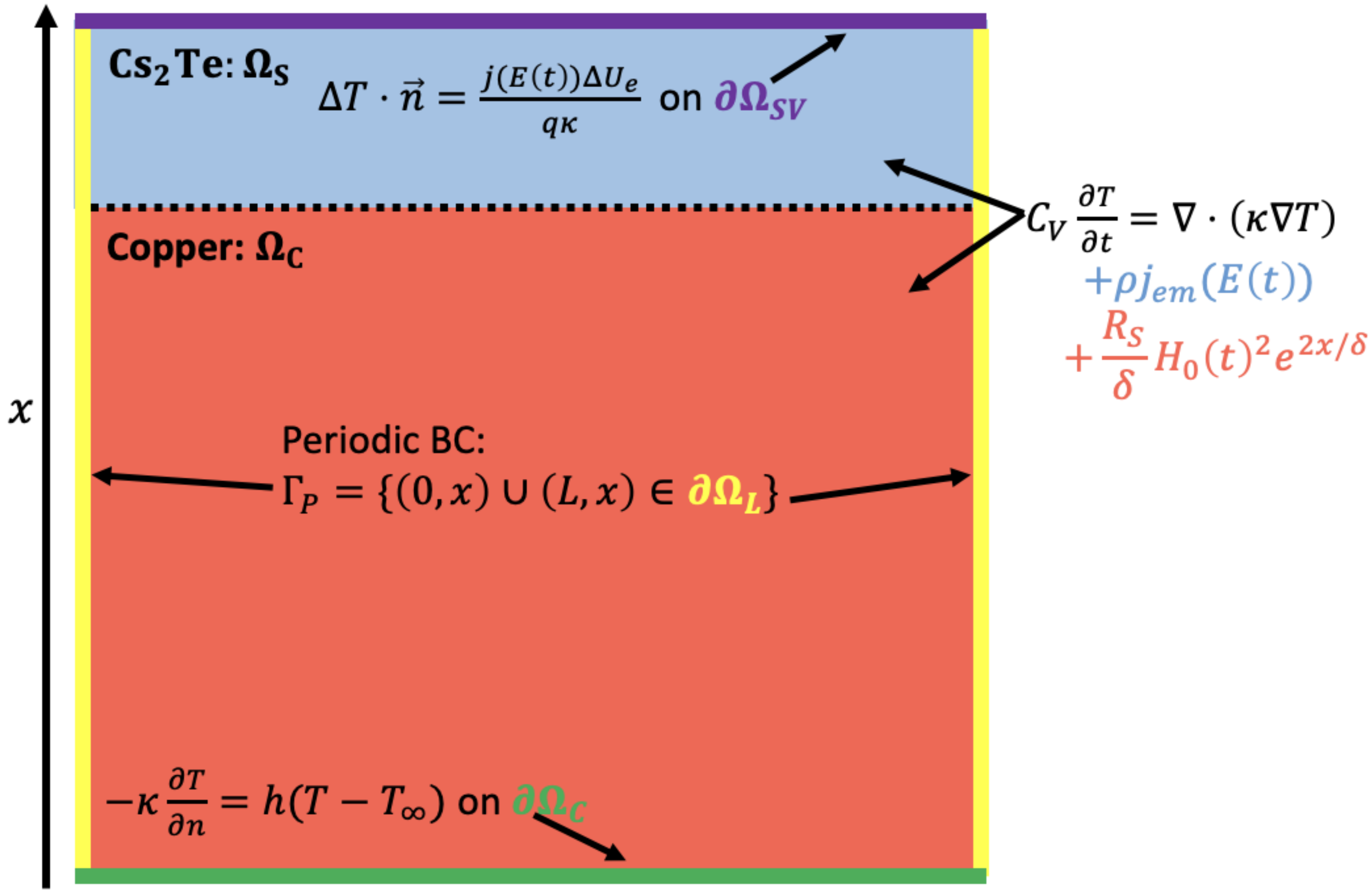
- Current-density Saturation in semiconductor
- Strong Deviation from classical FN equation in high-field regime
    - $1.54 * 10^6 * 10^{4.53\phi^{-0.5}} [\boldsymbol{E_{local}}]^2 Exp(-\frac{6.53*10^9*\phi^{1.5}}{\boldsymbol{E_{local}}})$
    - FN equation predicts that current increases exponentially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



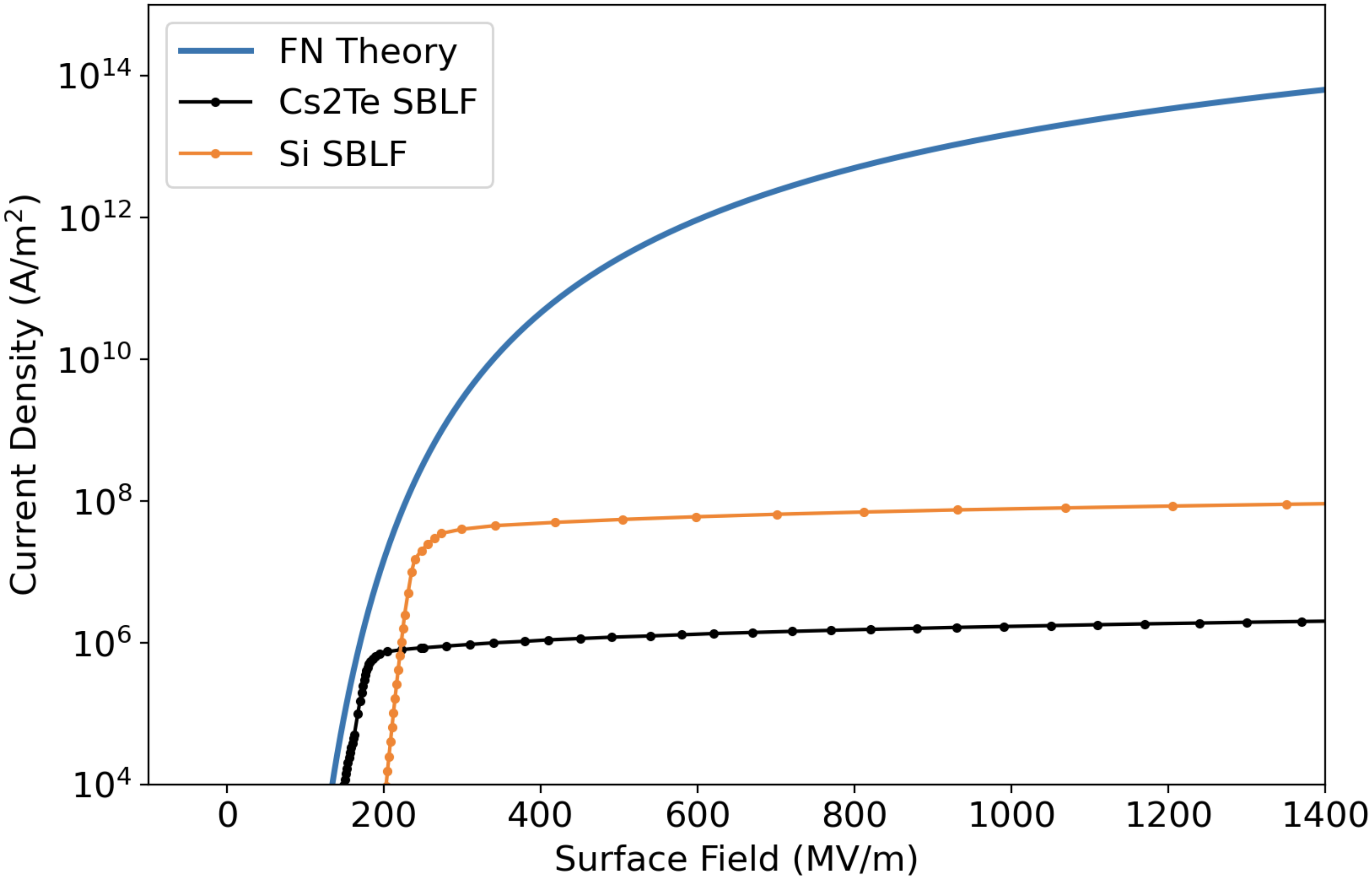
Journal of Applied Physics **125**, 205303 (2019); https://doi.org/10.1063/1.5085679

Simulation Setup

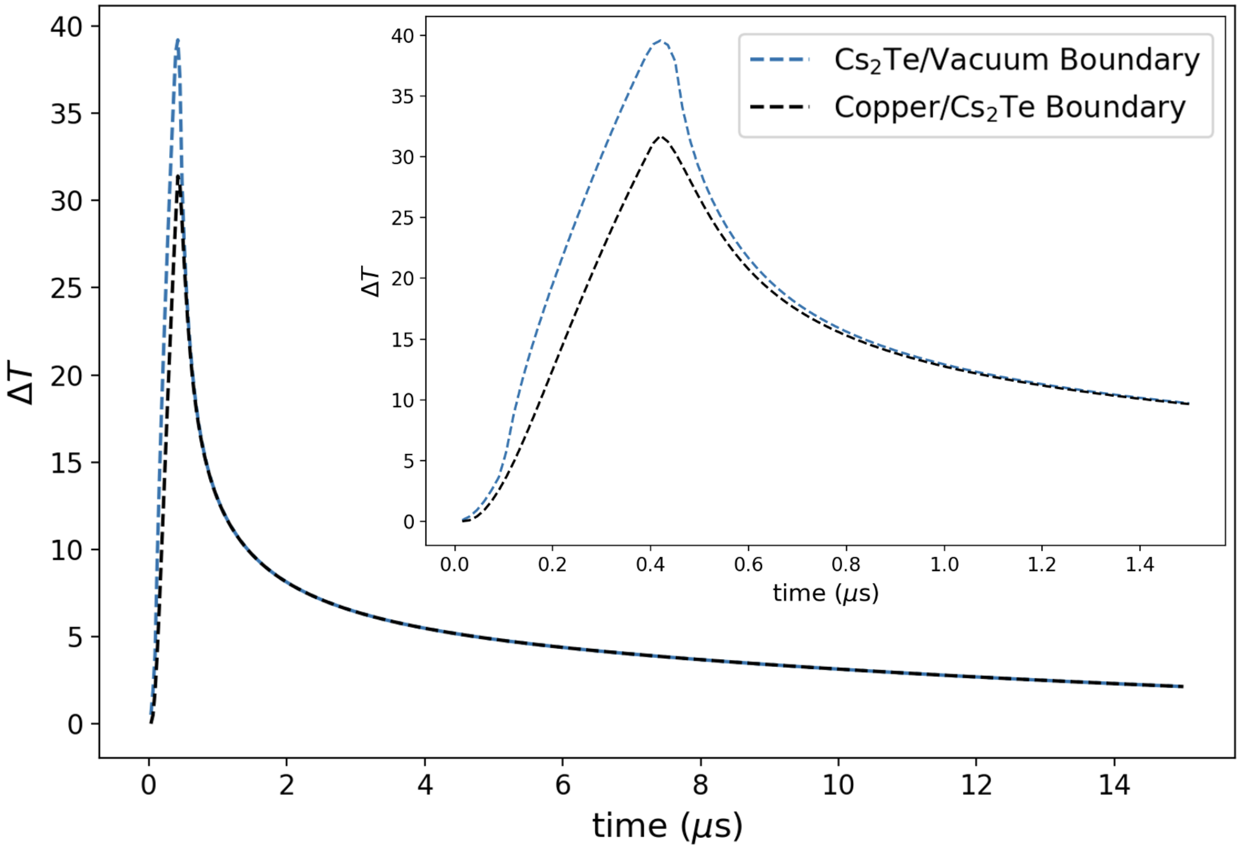
- Subdomains
  - Cs_2Te: Ω_S 50nm
  - Copper: Ω_C 50μm-10mm
- Heat Diffusion Eq:
  - $C_V \frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} + f(x,t)$
    - $f(x,t) = \frac{R_s}{\delta} |H_0(t)|^2 e^{-2x/\delta}$ on Ω_c
    - $f(x,t) = \rho j(E(t))^2$ on Ω_S

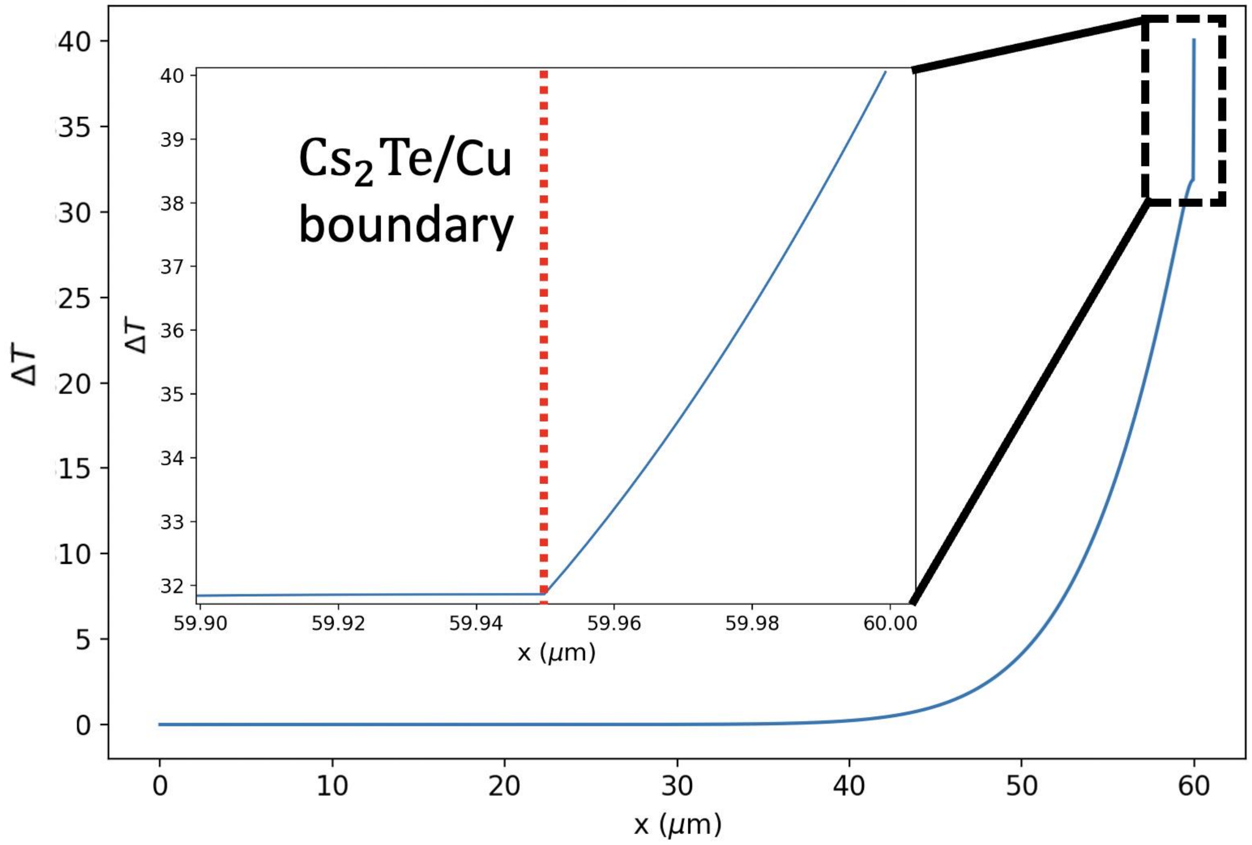


Cs_2Te Field Emission characteristics



Single Pulse Heating Behavior

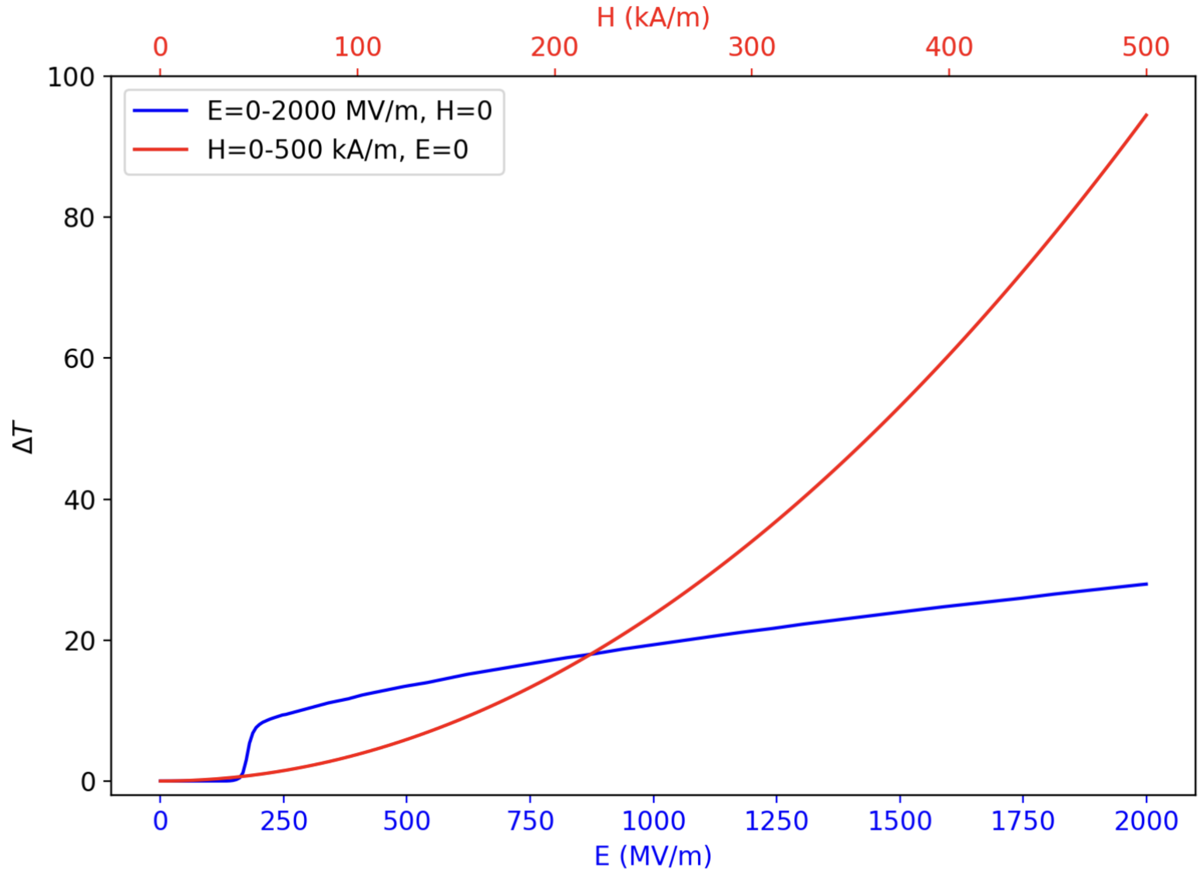




E vs H field Contribution Comparison

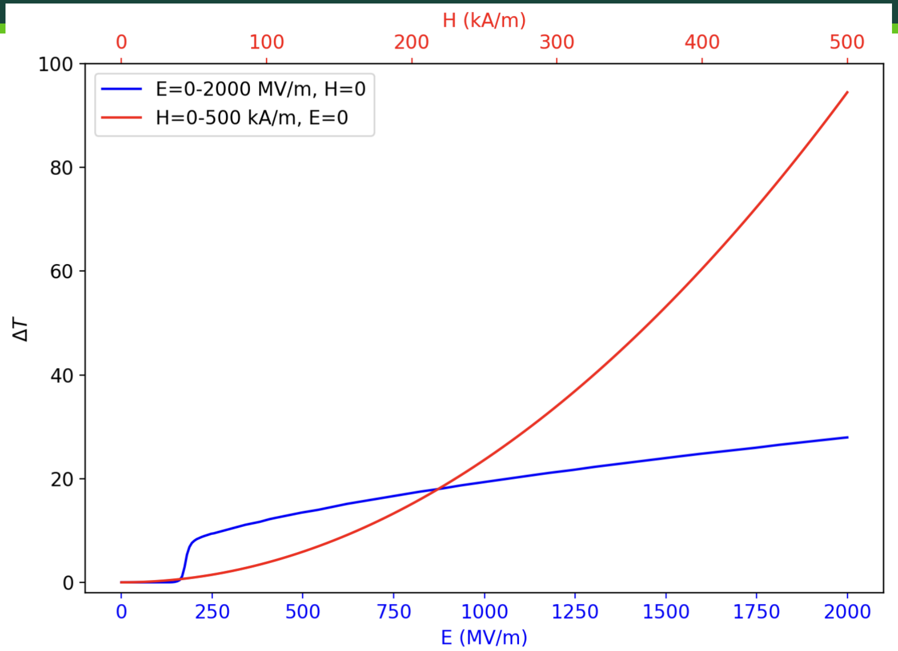
1. Keeping E=0 V/m while varying the H field
2. Keeping H=0 A/m while varying the E field

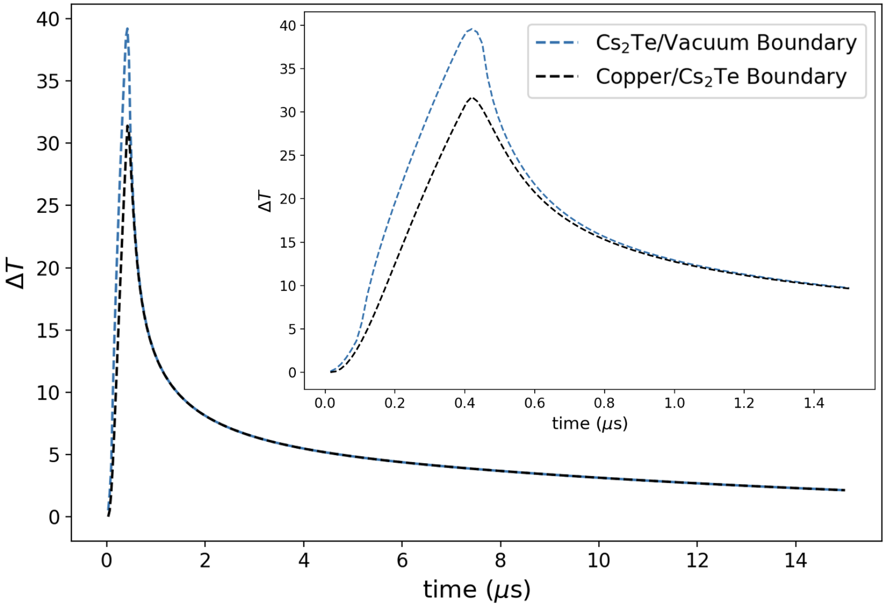
- Notes the maximum temperature during a pulse
- Within a reasonable range of surface EM fields, we see here that magnetic field contributes to much larger heating effect
  - Quadratic relation to H field
  - E field effect saturates due to current saturation



1D heating analysis

- Field Emission
  - Current Saturation: insufficient current for meaningful heating to take place for relevant range of parameter
- Pulsed Heating
  - Comparatively Larger heating expected
- Single Pulse:
  - $\Delta T \approx 40$ K
  - Enough heating to consider thermal stress induced surface evolution
- Multiple Pulse:
  - $\Delta T \approx 60$ K
  - Again, enough heating to consider surface evolution



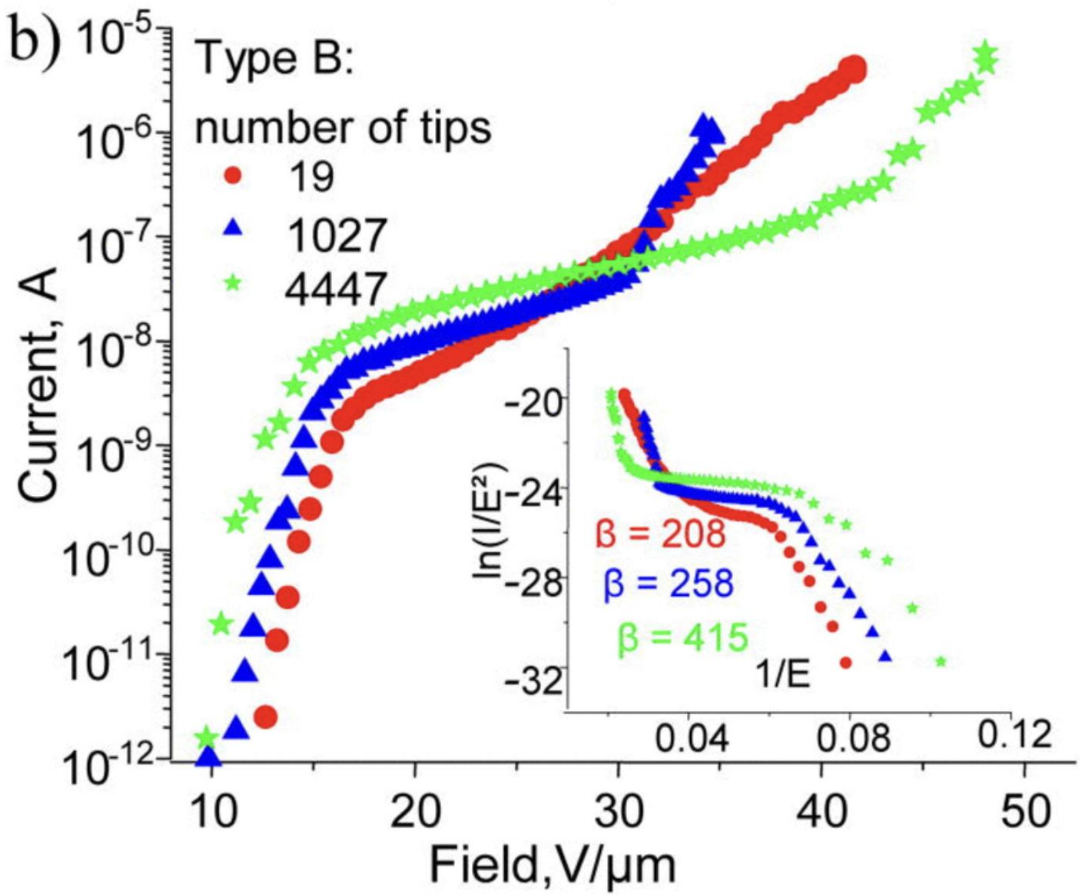


Discussion: dielectric breakdown?

- Potential regime beyond the saturation
- Johnson-Figure-of-Merit (JFOM)
  - Characterizes the material's suitability for high power and high frequency application

$$\mathrm{JFOM} = \frac{E_{br} \cdot v_{sat}}{2\pi},$$

  - For semiconductor thin-film, operation near 300 MV/m might be encroaching to this limit



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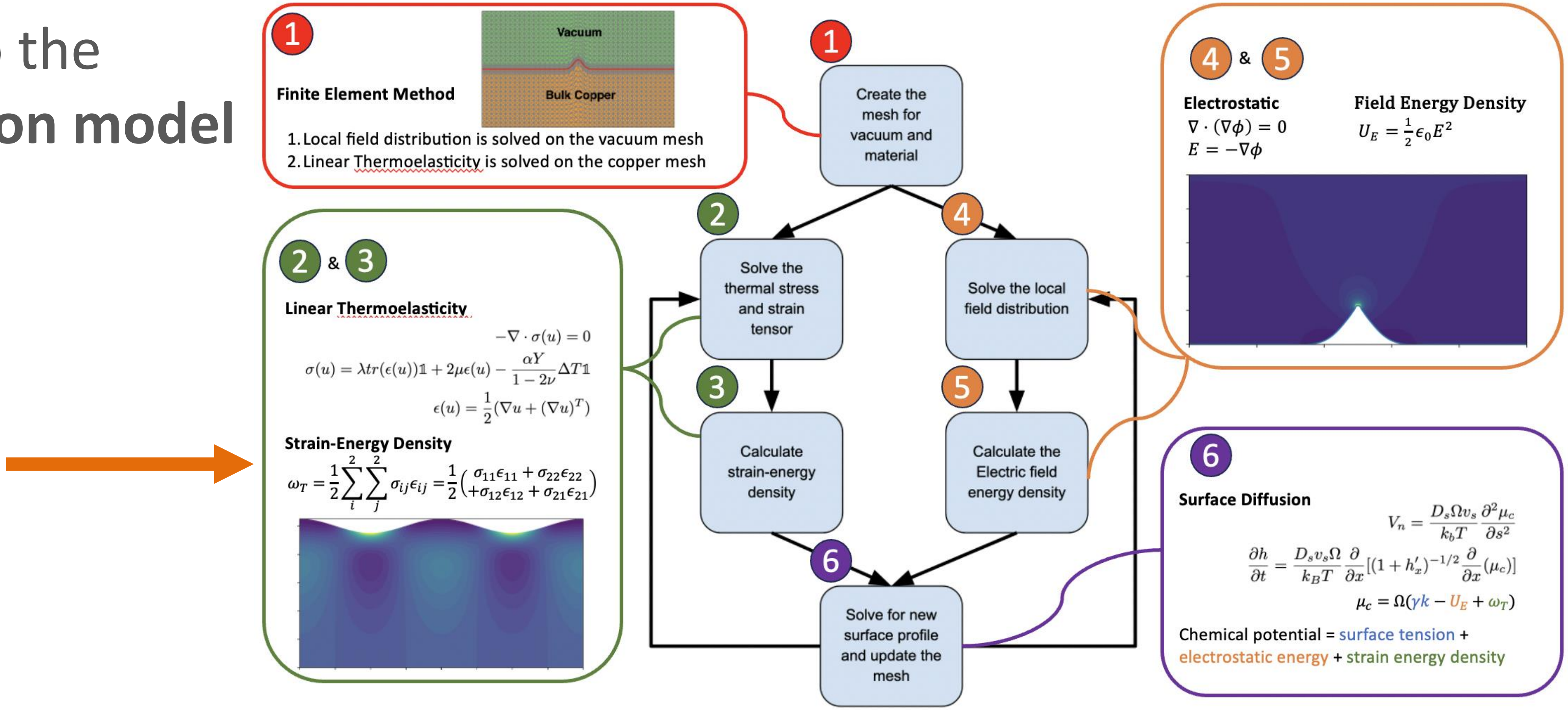
Semiconductor Heating:

- Couple back to the **surface diffusion model**



Self-consistently model Electrodynamic of Cs_2Te in 2D

- Drift Diffusion model

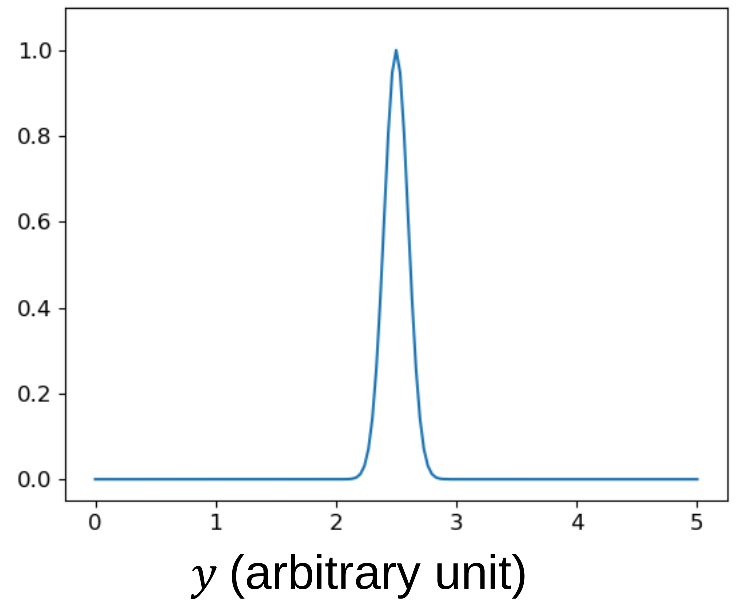
$$\nabla \cdot (\varepsilon \nabla \Phi) = -q(n - p + N_d - N_a) \qquad \mathbf{J}_n = -qD_n \nabla n + qn\mu_n \mathbf{E}$$

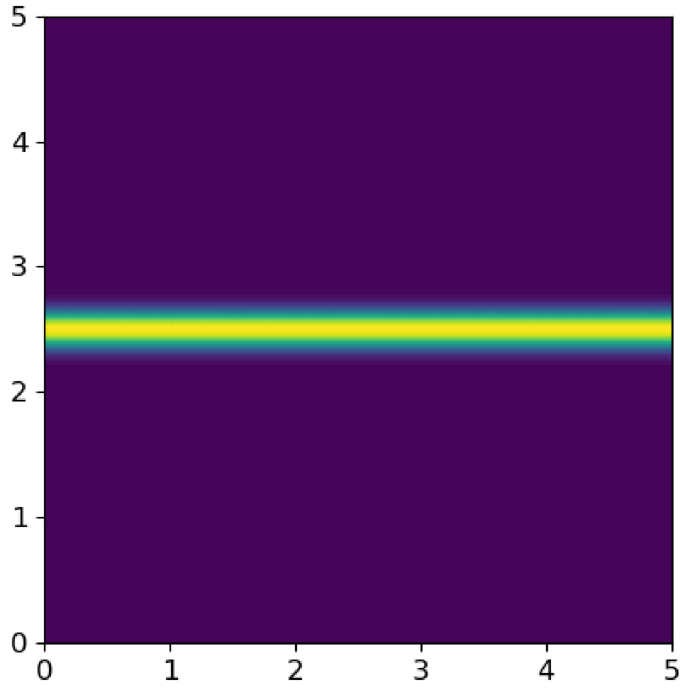
$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J}_n = G_n - R_n \qquad \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{J}_p = G_p - R_p \qquad \mathbf{J}_p = -qD_p \nabla p + qp\mu_p \mathbf{E}$$

- Final Variational form for coupled electron transport
- $\int \frac{n^{m+1} - n^m}{\Delta t} v_n dx = -q \int (\mu_n n^{m+1} E^{m+1} + qD_n \nabla n^{m+1}) \nabla v_n dx$

Future work: Working progress 2d Toy model

- Only electron considered here
  - $\nabla^2\Phi = \frac{\rho}{\varepsilon}, \rho = -qn \quad \mathbf{J}_n = -qD_n\nabla n + qn\mu_n\mathbf{E}$
- Current out from top surface





Publications

Published

- Ryo Shinohara, et al. **“Thermal and electric field driven rf breakdown precursor formation on metal surface”** Physical Review Accelerator and Beams
- R. Shinohara, Soumendu Bagchi, Evgenya Simakov, Danny Perez, Sergey V. Baryshev, X. Ting, and S. V. Baryshev, “Heating of Cs2Te Photocathode via Field Emission and RF Pulsed Heating: Implication Toward Breakdown” JVST B
- E. Jevarjian, R. Shinohara, Sergey Baryshev, M. Schneider, “FEgen (v.1): Field Emission Distribution Generator Freeware Based on Fowler–Nordheim Equation” IEEE Transactions on Plasma Science
- M. Schneider, B. Sims, E. Jevarjian, R. Shinohara, T. Posos, T. Nikhar, et al. “Ampere-class bright field emission cathode operated at 100 MV/m” Physical Review Accelerator and Beams

Plan after graduation: post doc opportunity after graduation in Accelerator field (e.g. LANL)

Acknowledgement

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Questions?