Modeling of metallic interfaces under high electric fields for particle accelerators

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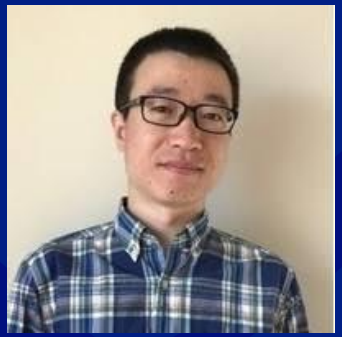
Acknowledgements:
Soumendu Bagchi, Ryo Shinohara, Gaoxue Wang, Sergey Barishev, Evgenya Simakov
LANL LDRD program

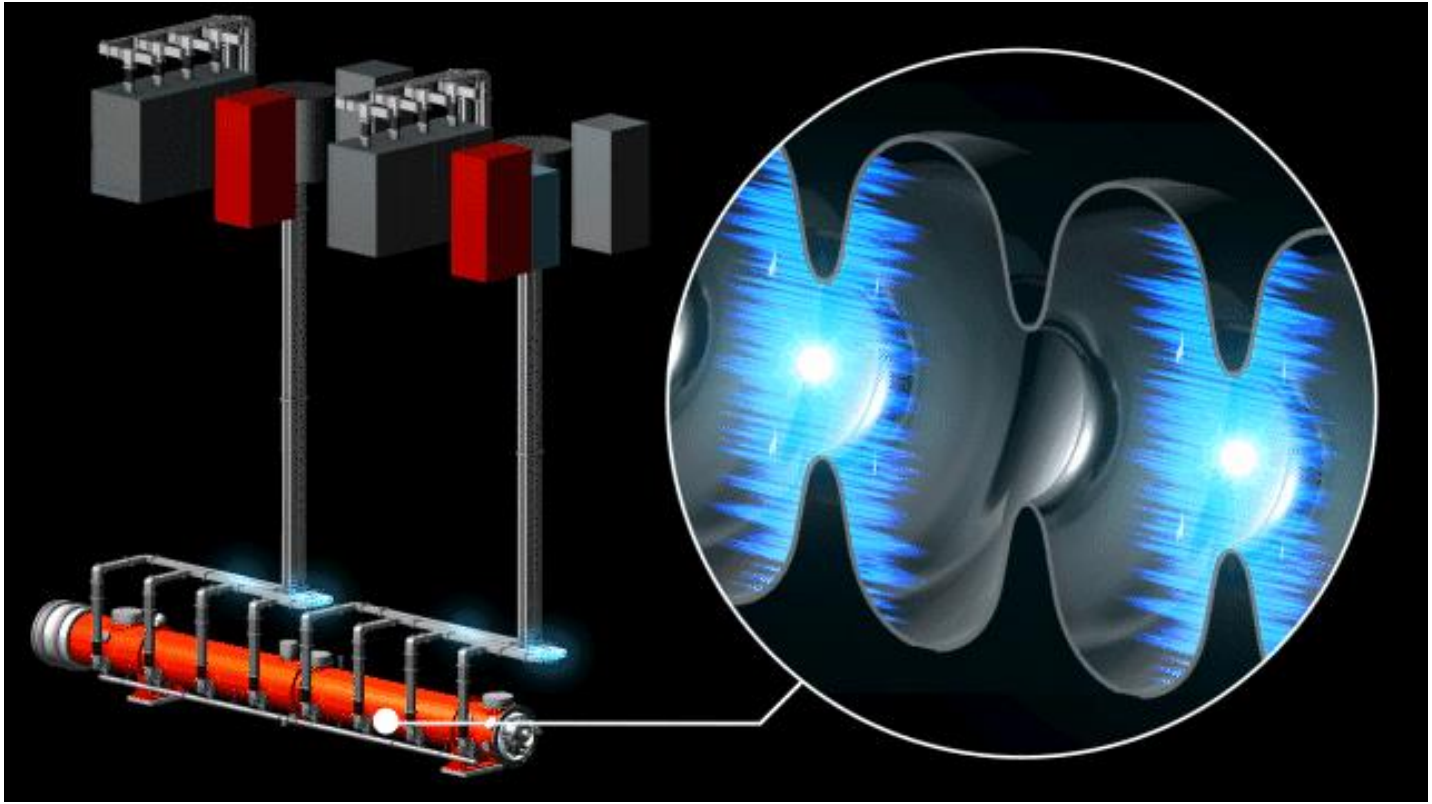
Ryo Shinohara

Soumendu Bagchi



Gaoxue Wang

Particle accelerators 101



Greg Stewart/SLAC National Accelerator Laboratory

Basic parameters

- **Average accelerating gradient – 100-200 MV/m**
- **Peak surface electric field – 200-400 MV/m**

- RF frequency – 10 GHz
- Pulse length – 100 ns
- Repetition rate – 100 Hz
- Input power – 50 MW
- Pulse energy – 10 J

- Cavity is usually made of Cu

The race to higher fields

Increasing accelerating fields is generally beneficial:

- Smaller size (medical, space applications)
- Lower cost (material, footprint)
- Higher energies

Limiting factors:

- Available RF power
- Multipacting: resonant electron–avalanche
- Losses: ohmic heating and thermal fatigue
- Vacuum breakdown

[Wuensch et al, arXiv:2502.03967]

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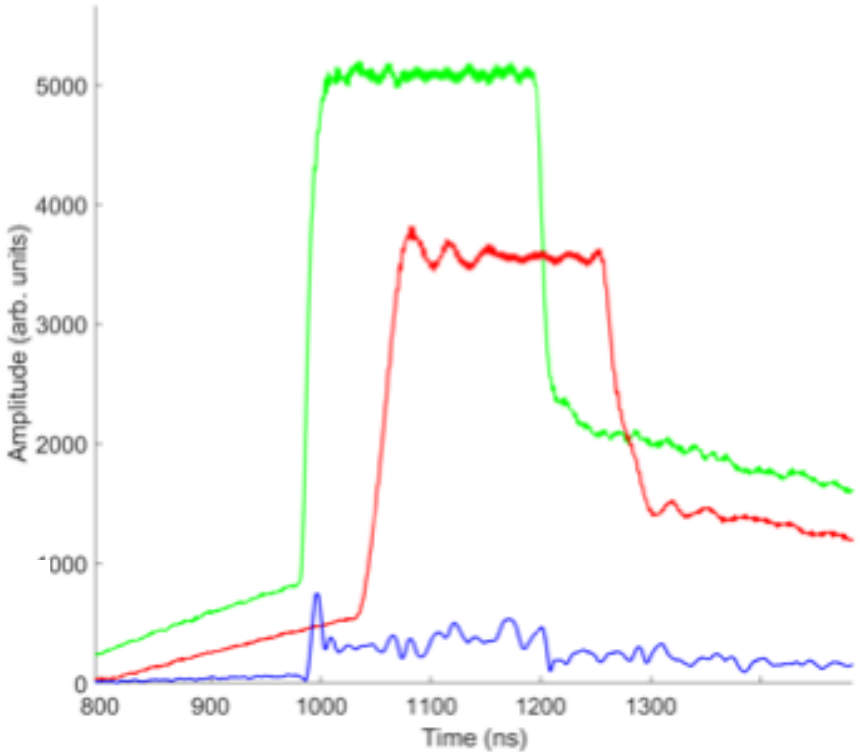
[Wuensch et al, arXiv:2502.03967]

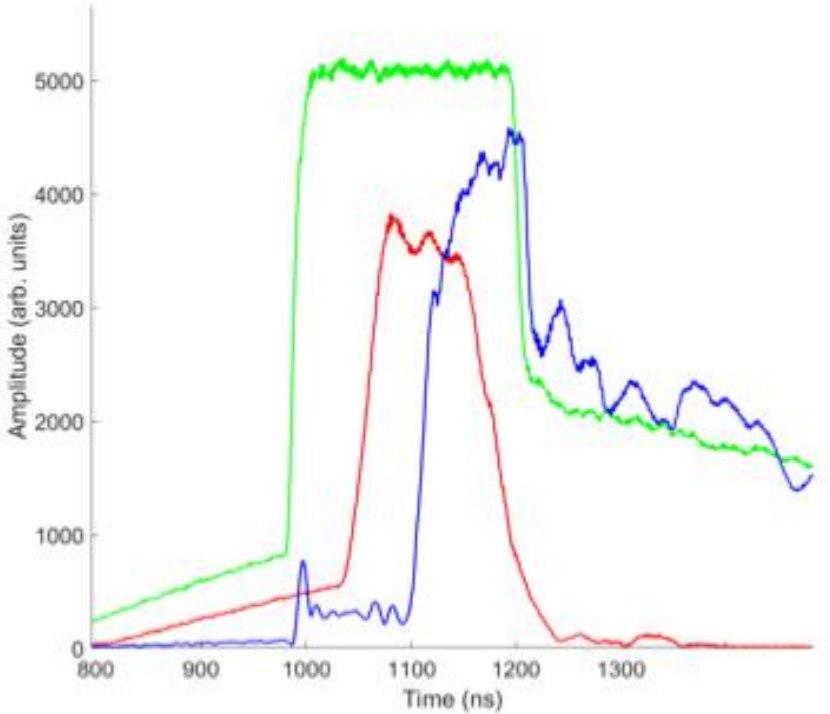
Breakdown for accelerator operators

Incident power
Transmitted power
Reflected power

Normal

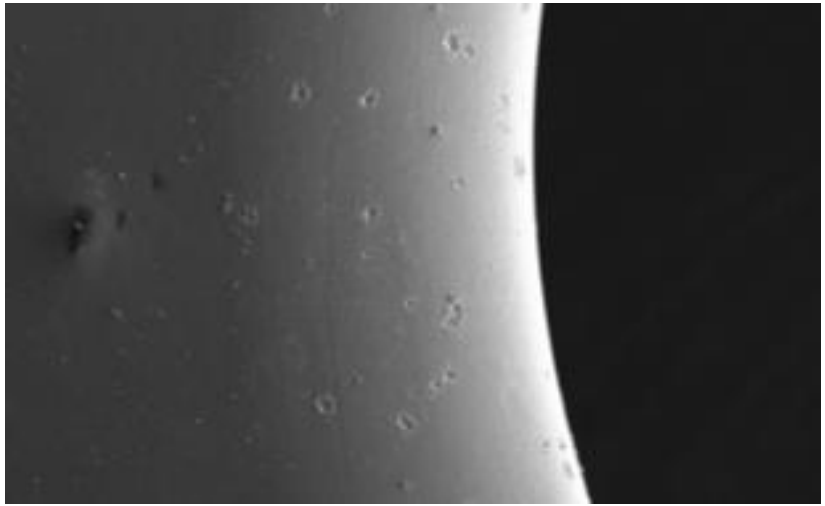


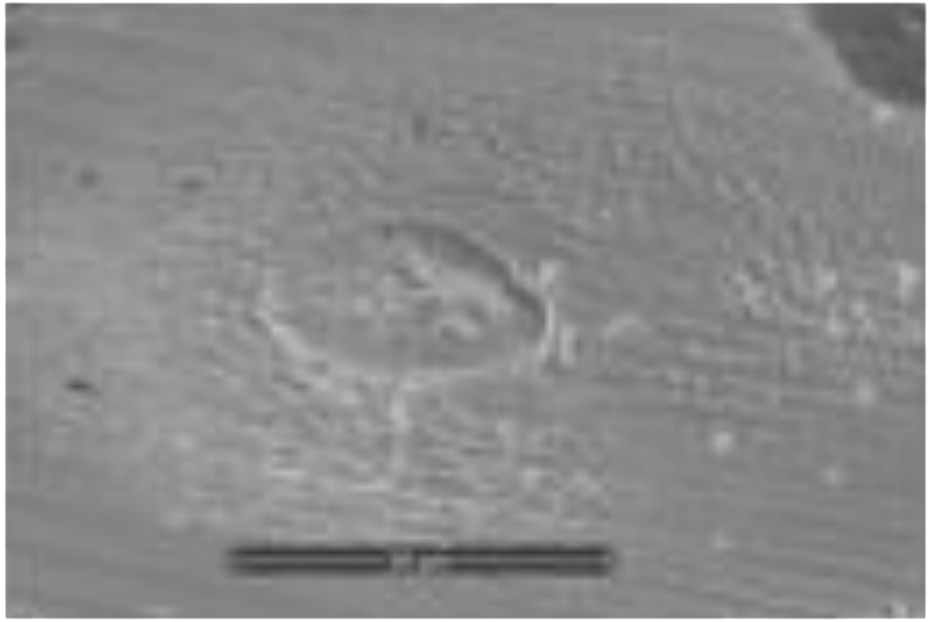
Breakdown



[Wuensch et al, arXiv:2502.03967]

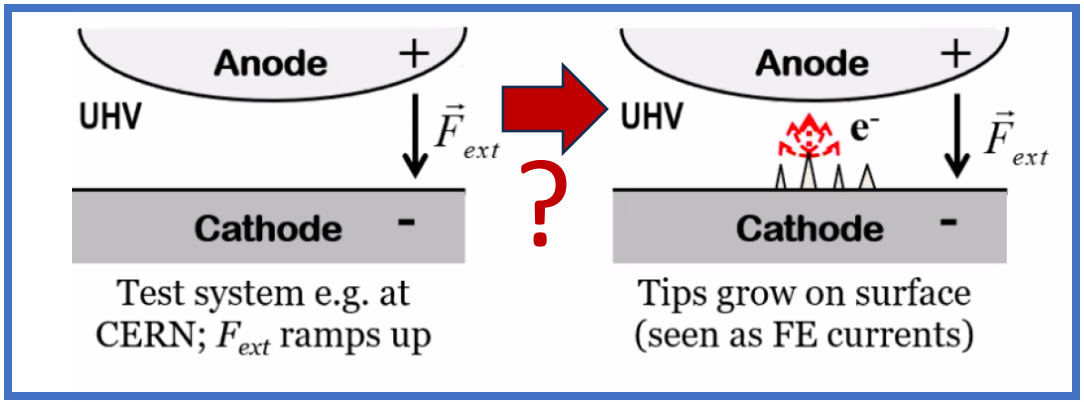
Breakdown for materials scientists

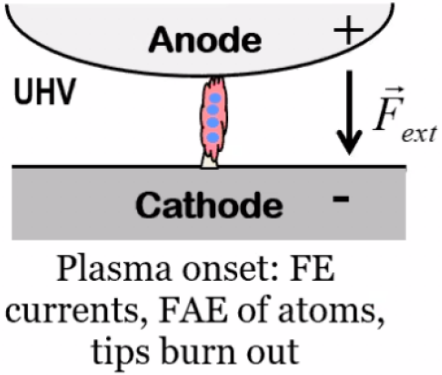


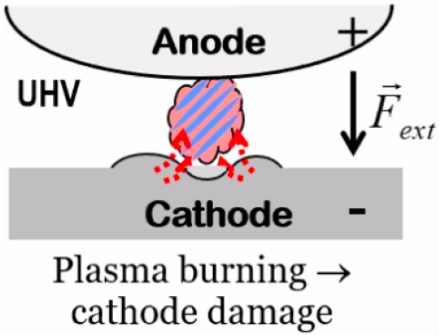


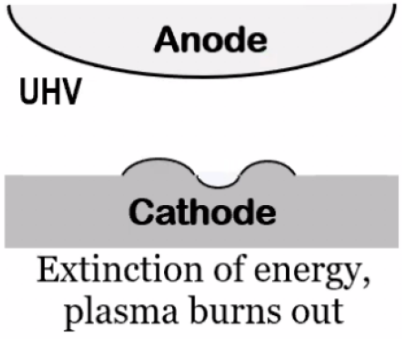
[Wuensch et al, arXiv:2502.03967]

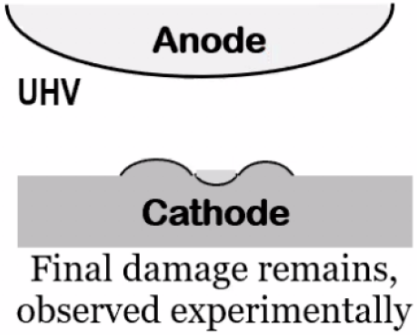
Breakdown: what do (we think) we know?





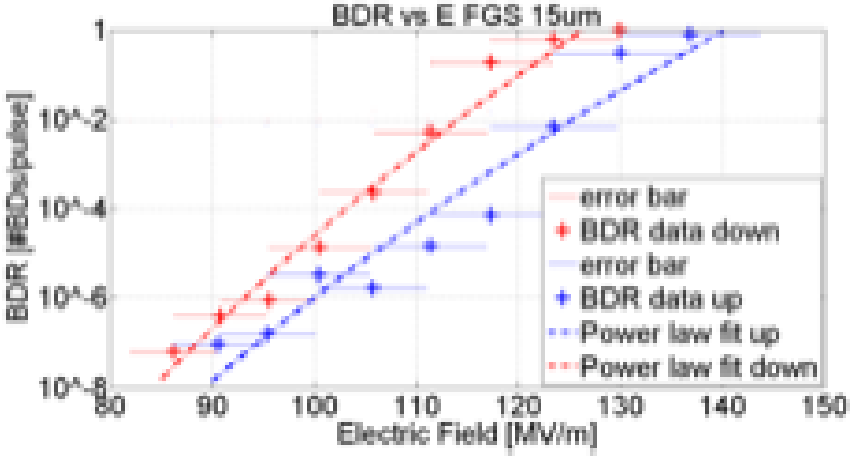


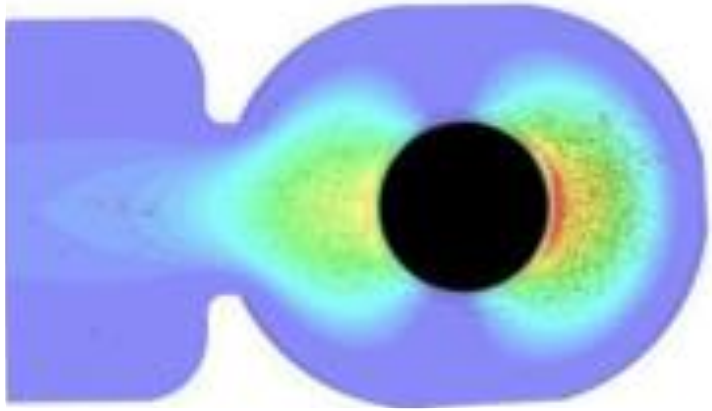




[Djurabekova et al. (2010)]

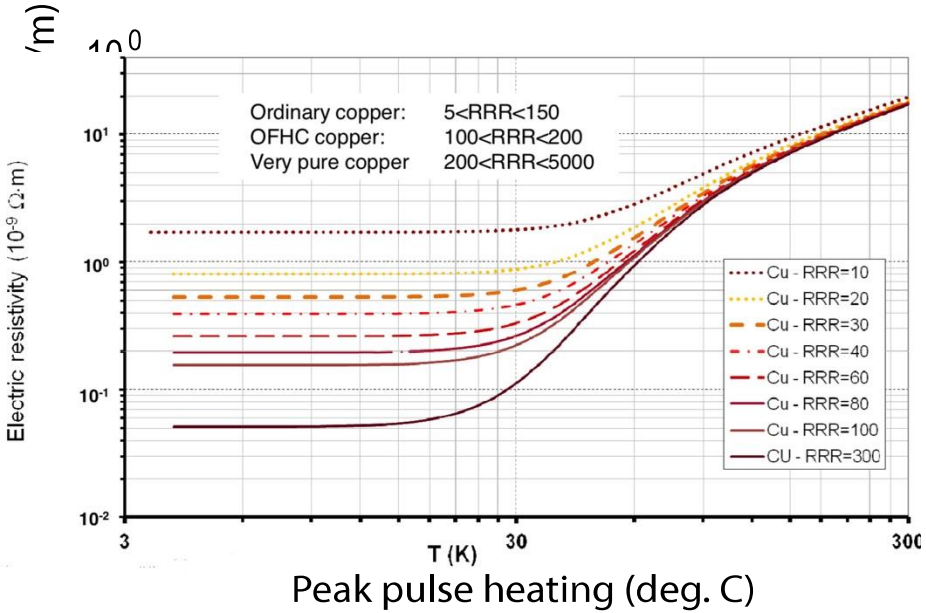
Possible driving force: Electric field





- Concentrates in high E-field regions (but not exclusively)
- Extremely steep field dependence ($E^{20\text{-}40}$)!

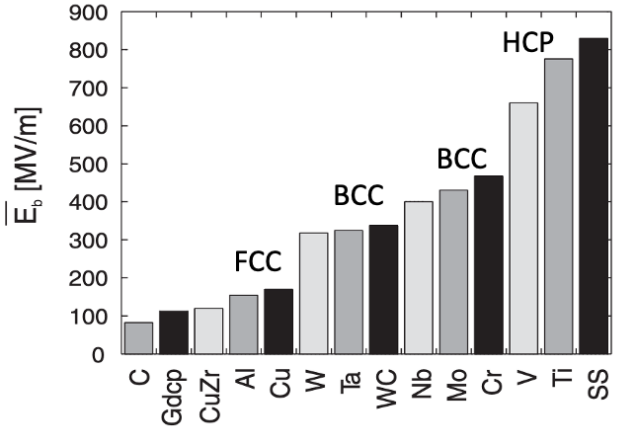
Possible driving force: RF Losses



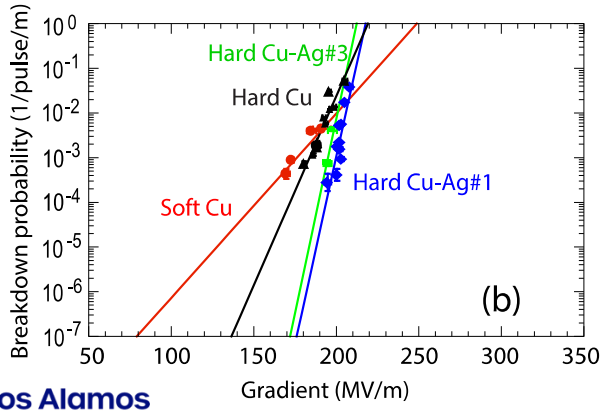
- RF pulses cause cyclic Joule heating near the surface (skin depth ~ μm)
- BDR scales with peak pulse heating
- Losses and BDR significantly decrease in cryogenic conditions

Vignette #1: Plastic-deformation induced roughening

[Descoeudres et al (2009)]



[Dolgashev et al (2021)]



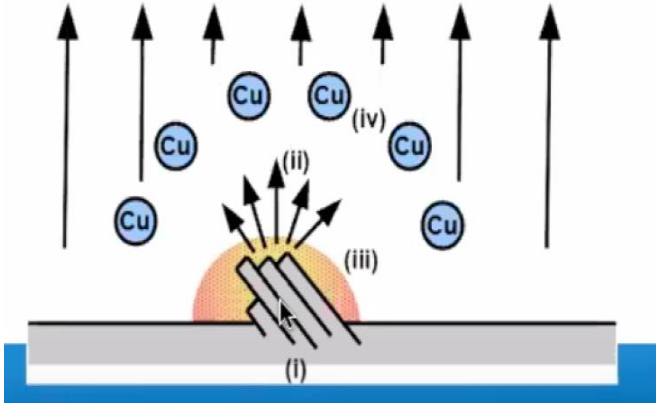
Material properties matter:

- Harder materials = lower BDR
- Processing matters (welding, …)

- Possible relevant physics:
  - **Plastic deformation**
  - **Dislocation motion/multiplication**
  - Microstructure
  - Fatigue
  - …

Vignette #1: Plastic-deformation induced roughening

- Runaway dislocation multiplication has been hypothesized as a breakdown precursor
- Current analytical models have yet to be demonstrated in simulations
- Goal: **assess dislocation-multiplication processes using molecular dynamics**



MD of metals under E field

- Conventional charge-equilibration (QEq):

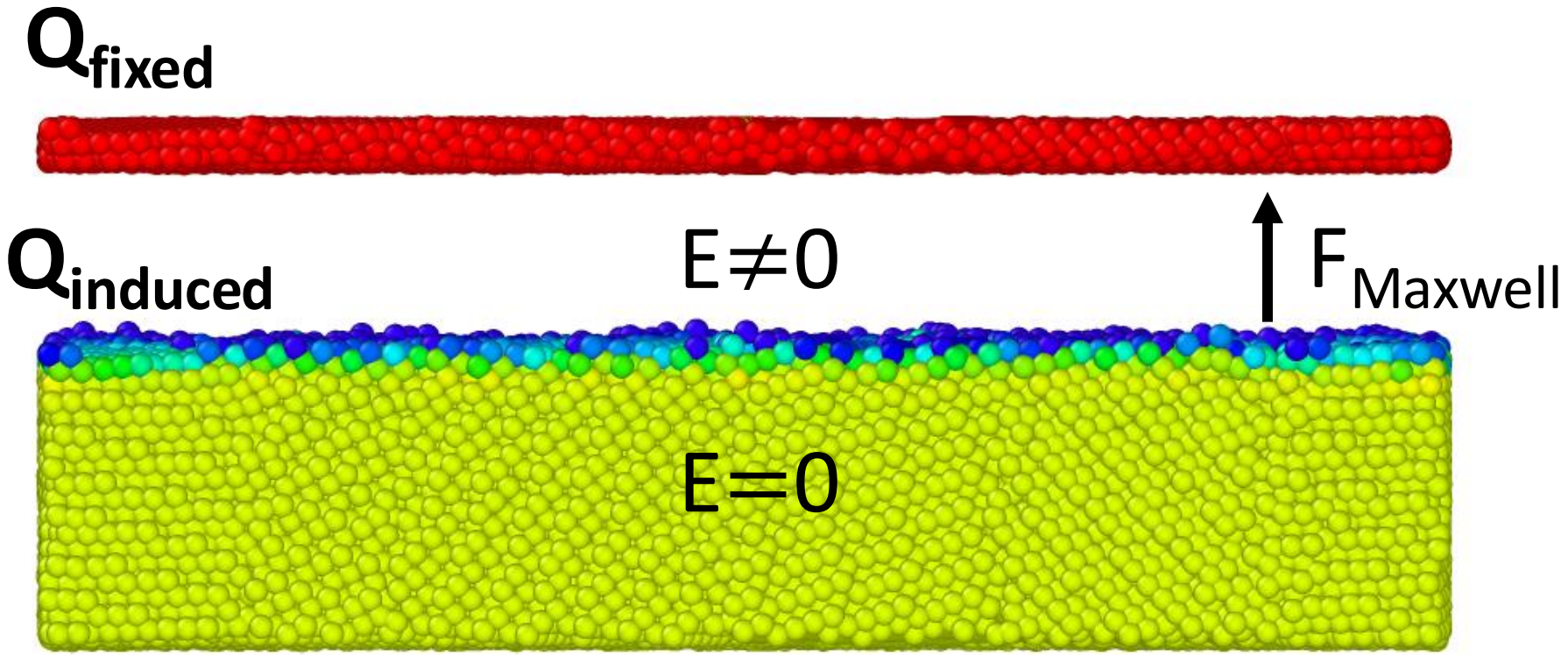
$$\min_{\mathbf{q}} \quad E_{\mathrm{ele}}(\mathbf{q}) = \sum_{i}^{N} \chi_i q_i + \frac{1}{2} \sum_{i,j}^{N} H_{ij} q_i q_j$$

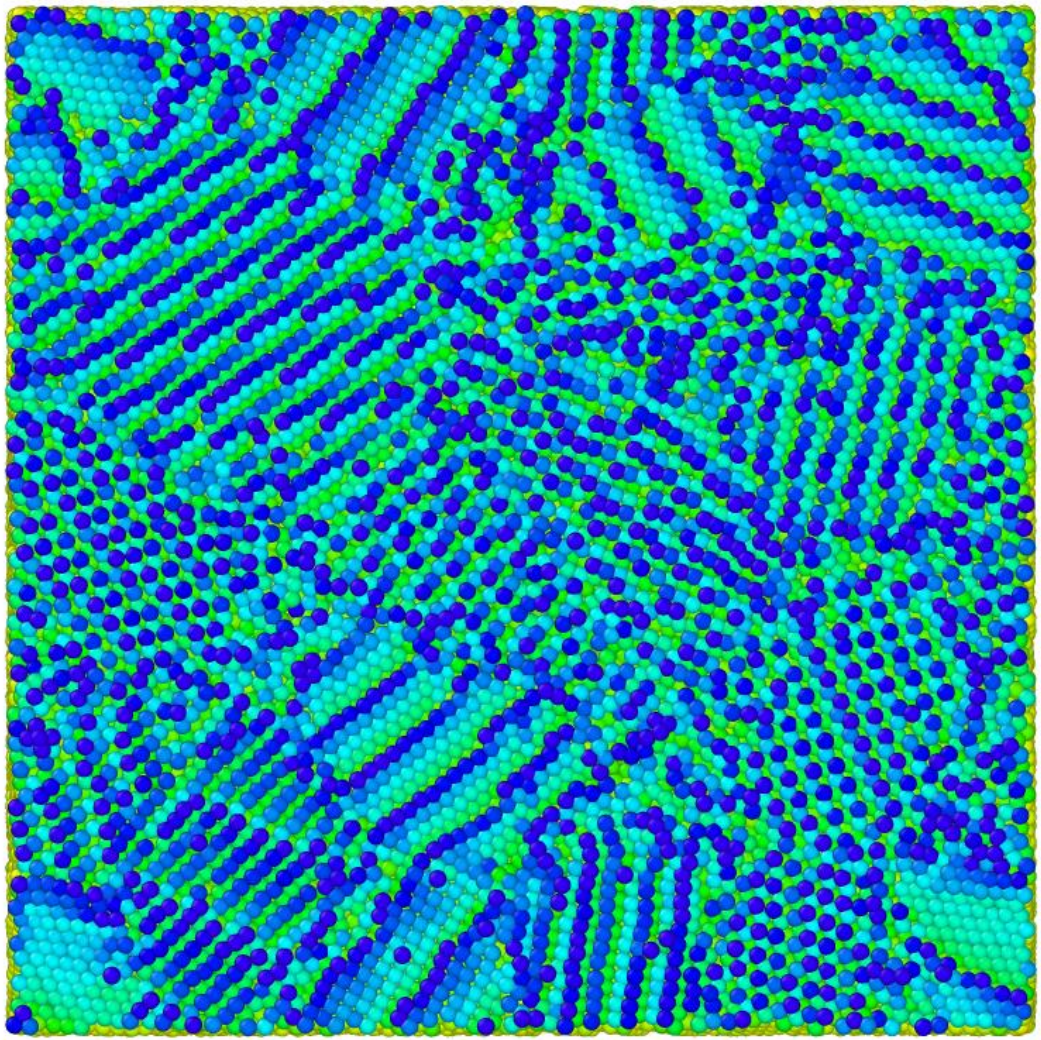
$$\text{subject to} \quad \sum_{i}^{N} q_i = 0$$

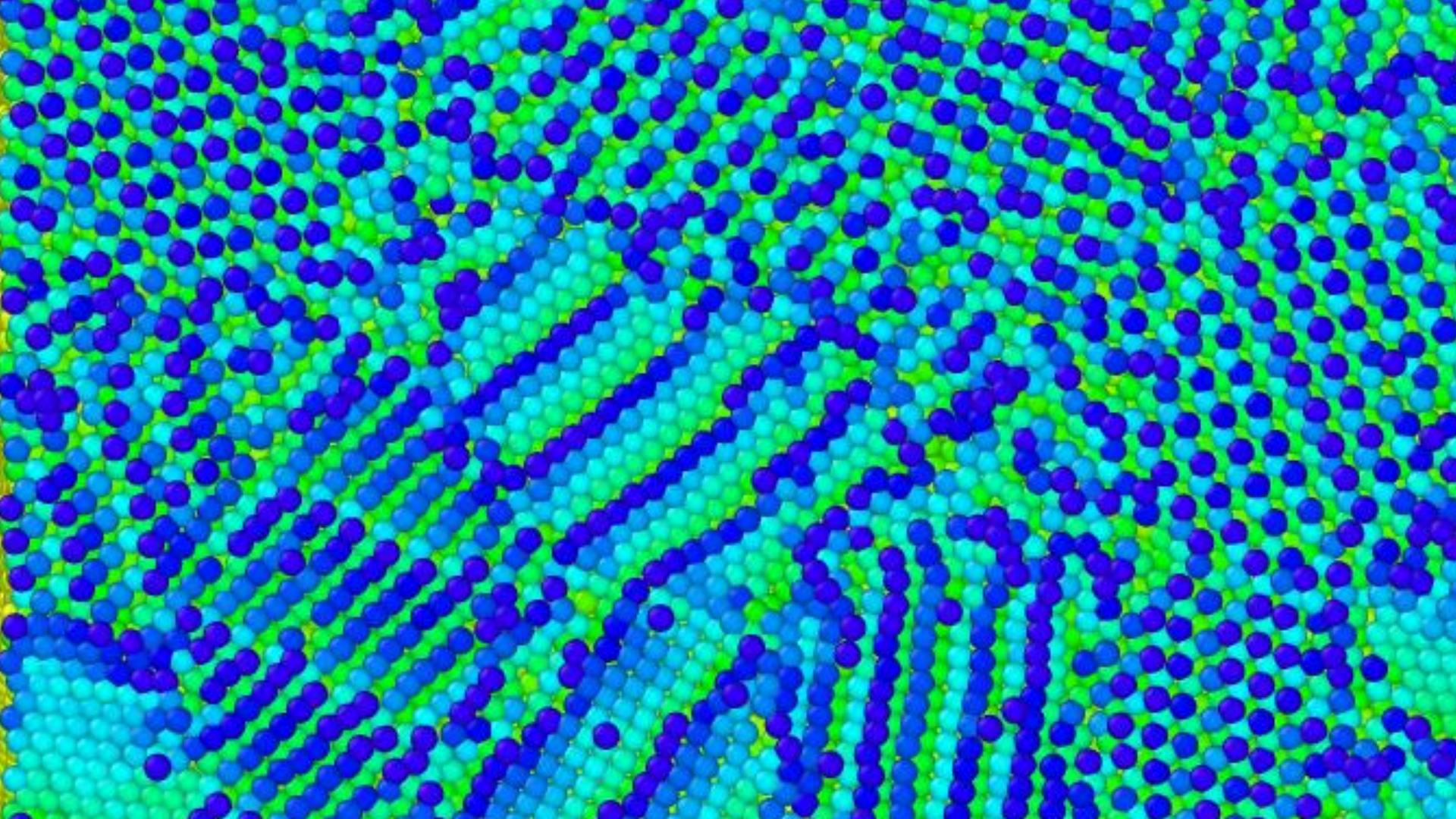
$$H_{ij} = \delta_{ij} \eta_i + (1 - \delta_{ij}) \cdot F_{ij}$$

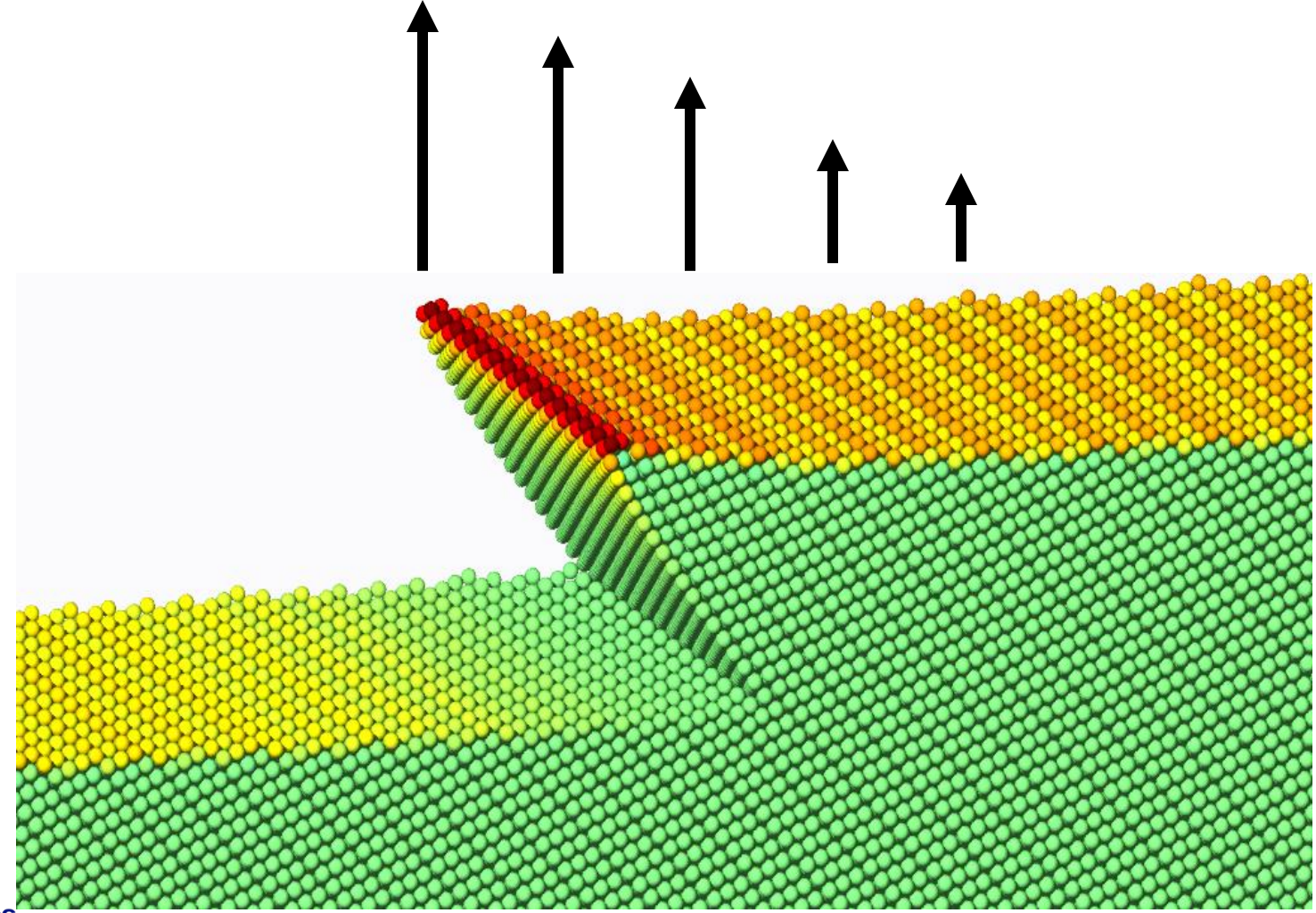
- Reasonable description of metals. Natural coupling to external fields
- Caveat: need untruncated Coulomb interactions

[Rappe and Goddard, 1991]


Q_{fixed}
$Q_{induced}$
E≠0
$F_{Maxwell}$
E=0

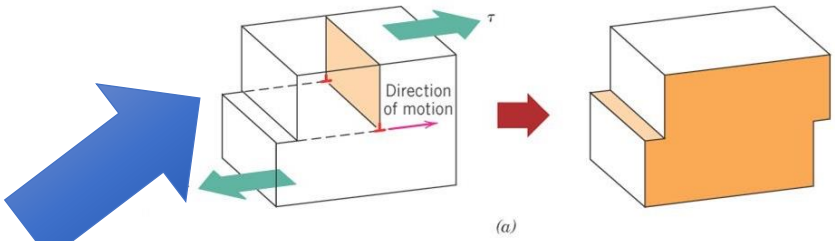


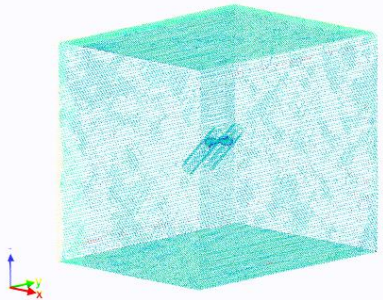




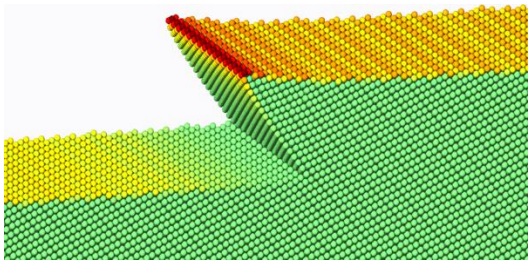
Runaway dislocation emission!

Surface features



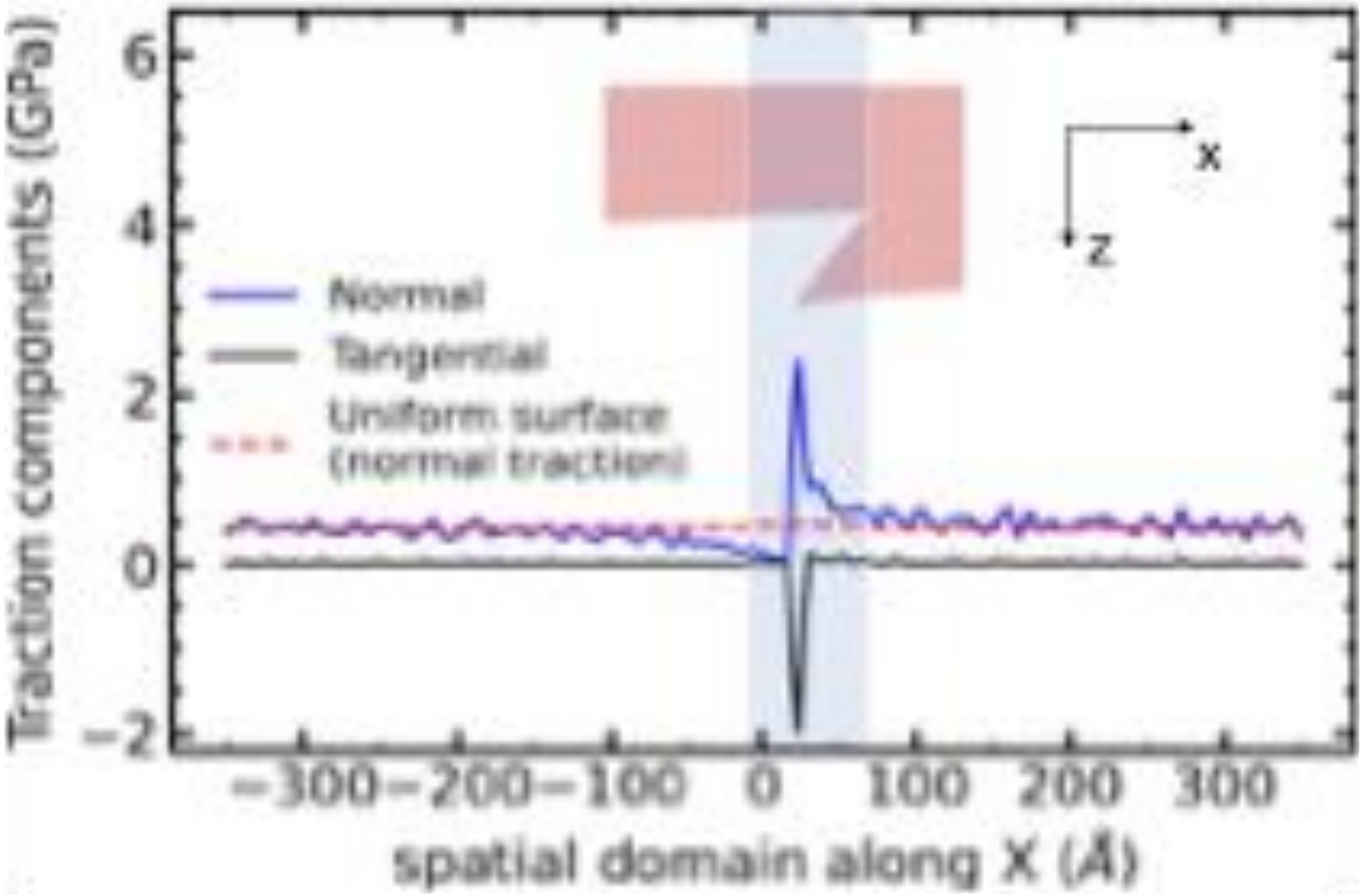


Plastic deformation



Charge/stress concentration due to E

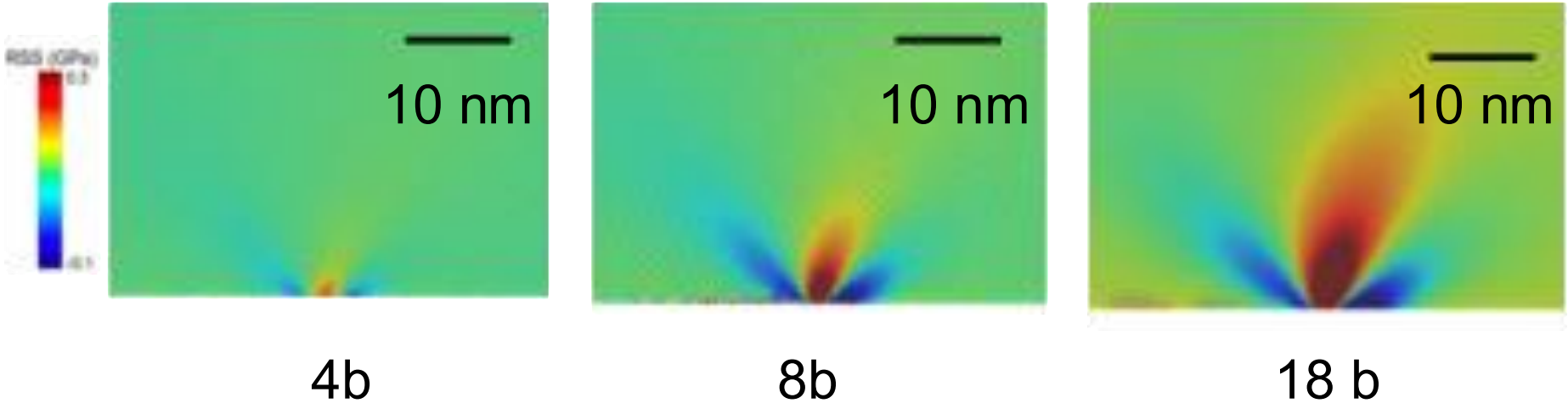
[Bagchi, Perez (2022, 2025)]



10 GV/m, step height = 18 b

Field/step coupling induces resolved shear stresses

10 GV/m

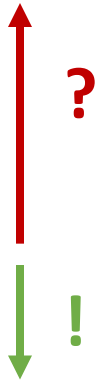


4b 8b 18 b

Increasing step height

Runaway dislocation emission?

Electric field	Maxwell stress on a flat surface	Critical Frank-Read source length
10 MV/m	400 Pa	50 mm
100 MV/m	40 KPa	0.5 mm
1 GV/m	4 MPa	5 μm
10 GV/m	400 MPa	50 nm



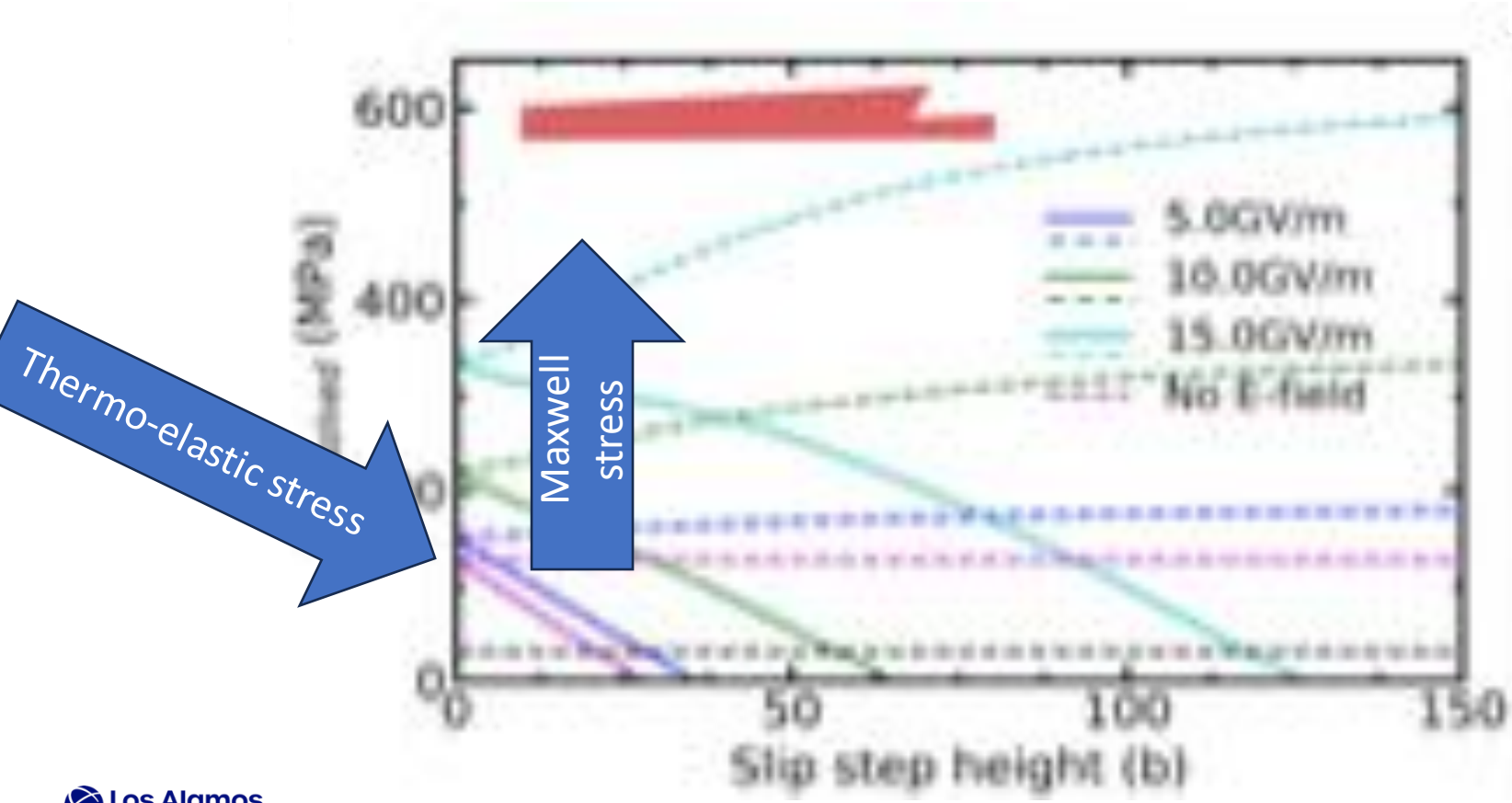
- Yield strength of annealed Cu: ~30 MPa
- Peierls stress of Cu: ~0.3 MPa

Runaway dislocation emission?

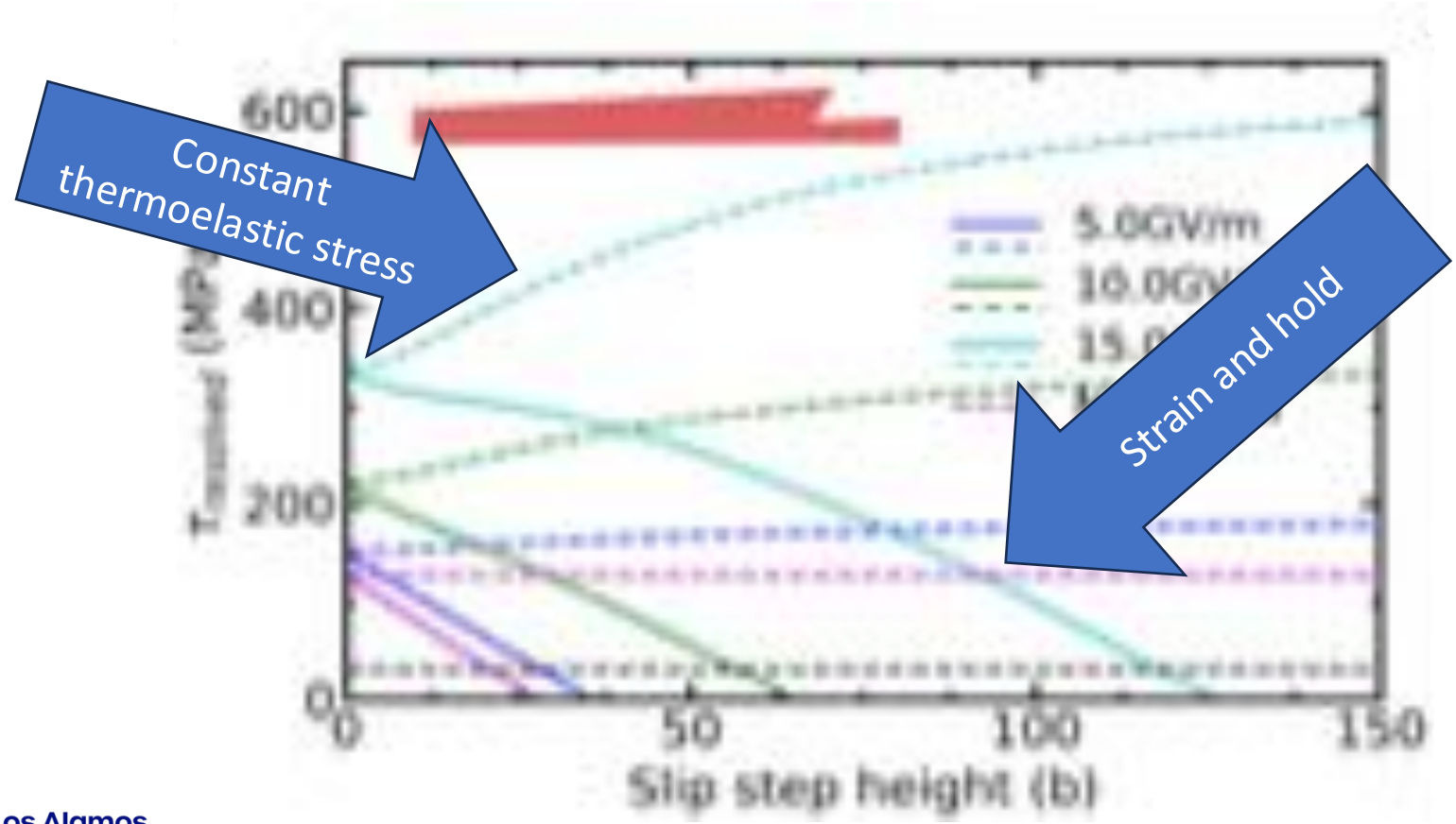
ΔT rise	Thermo-elastic stress
10 K	16 MPa
20 K	32 MPa
40 K	64 MPa
80 K	128 MPa

- Yield strength of annealed Cu: ~30 MPa
- Peierls stress of Cu: ~0.3 MPa

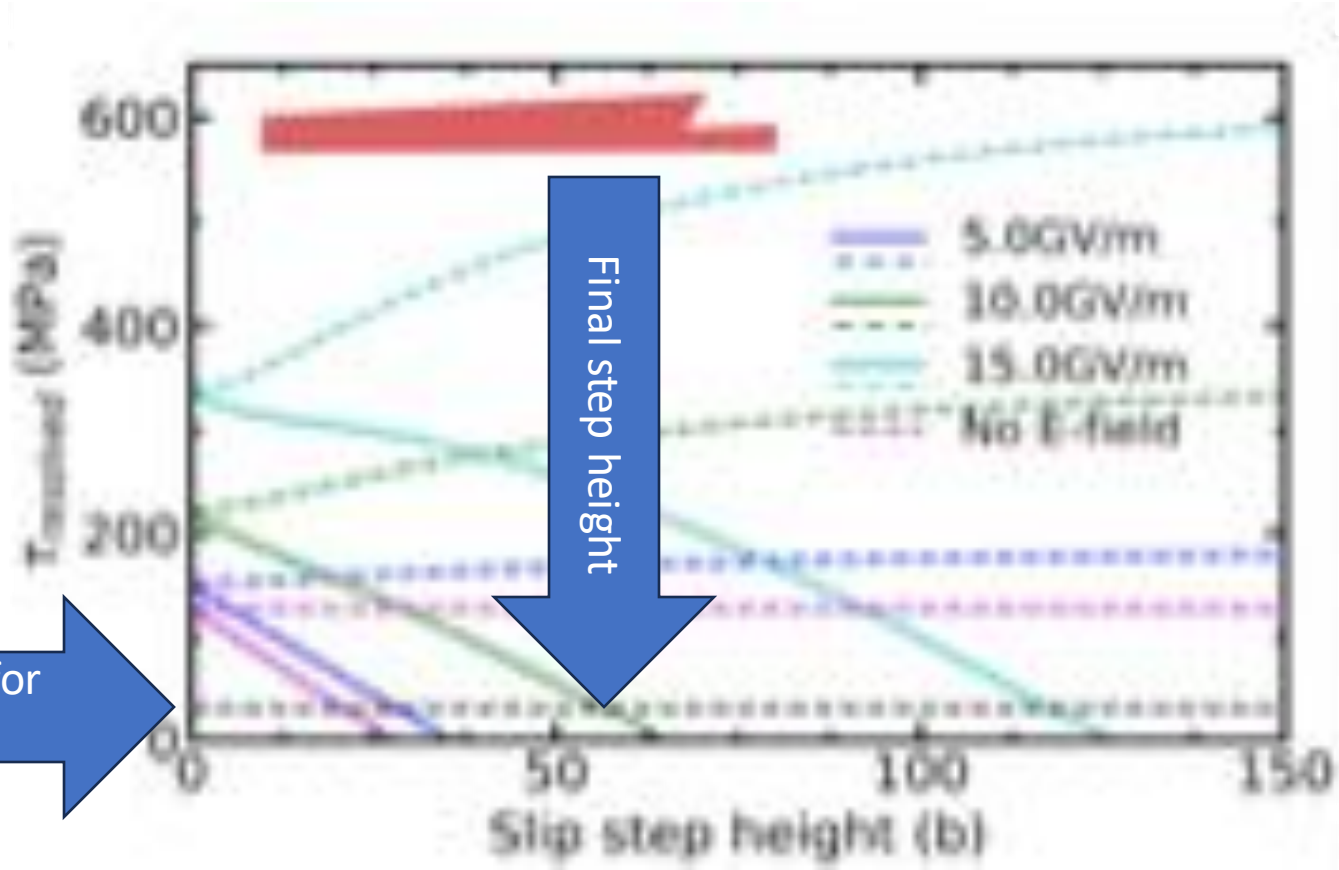
Dislocation emission at ΔT=80K



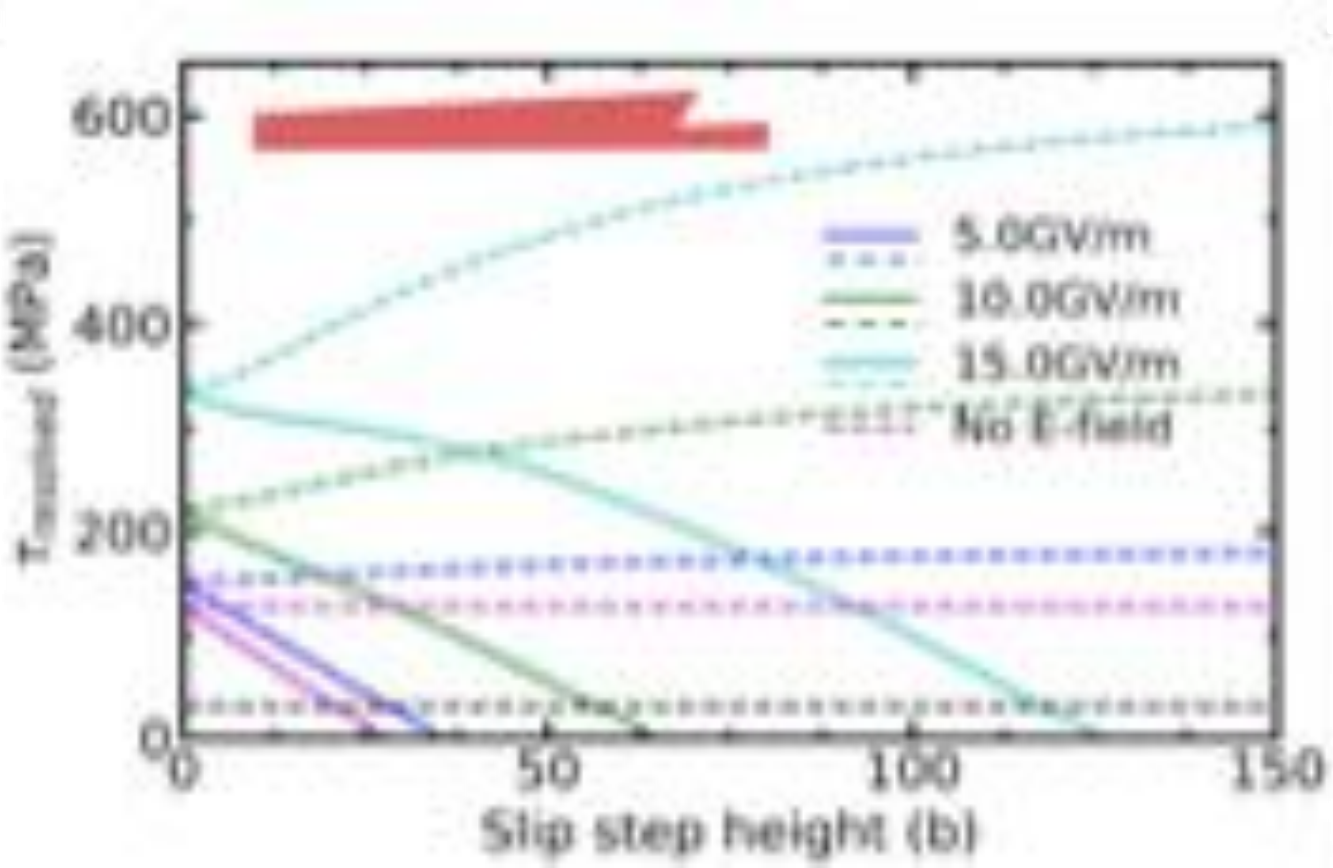
Dislocation emission at ΔT=80K



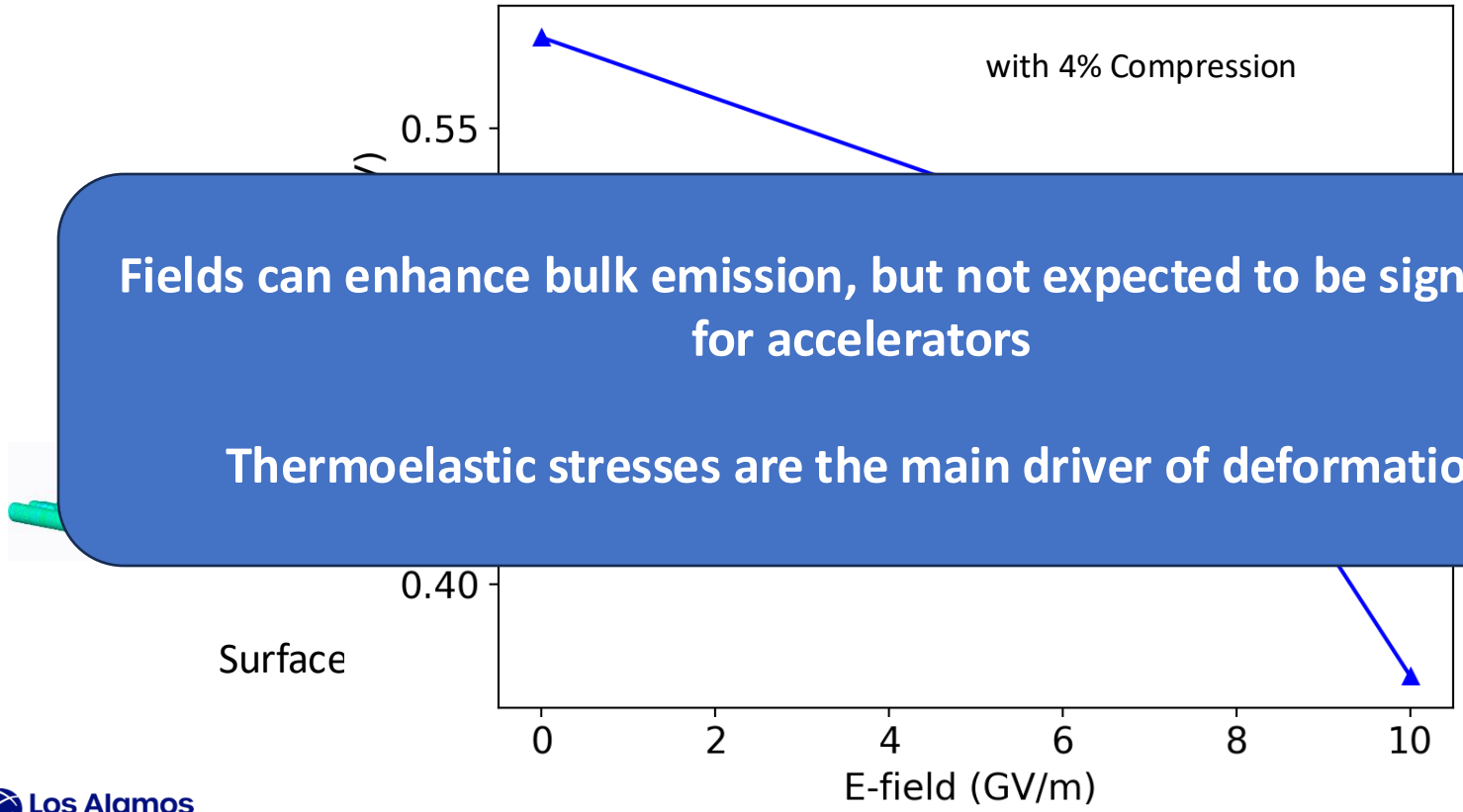
Dislocation emission at ΔT=80K



Dislocation emission at ΔT=80K



Surface dislocation multiplication

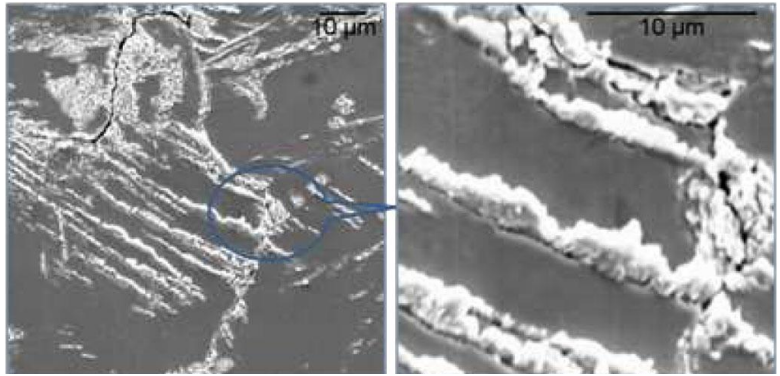


Fields can enhance bulk emission, but not expected to be significant for accelerators

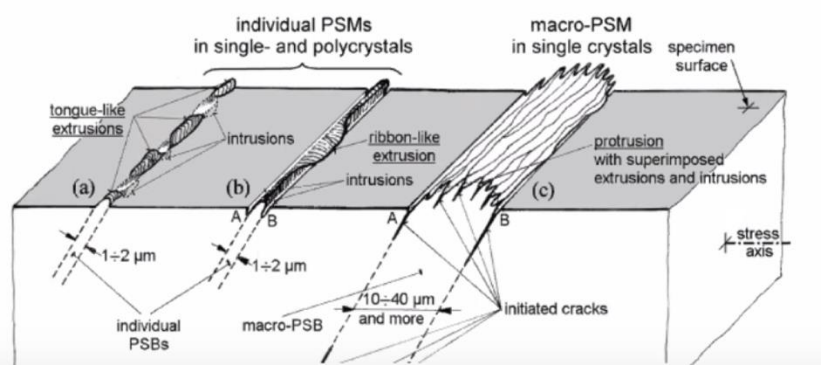
Thermoelastic stresses are the main driver of deformation

Vignette #1: Plastic-deformation induced roughening

- LARGE electric fields can enhance dislocation emission
- **Unlikely to be relevant for breakdown precursor formation**
- **Could activate once a precursor is formed by some other means**
- Thermal cyclic fatigue is a prime candidate.



[Laurent, Tantawi, Dolgashev et al. (2011)]



[Man et al. (2009)]

Vignette #1.1: Can we design better materials?

- **Design principle #1: minimize RF losses**
- **Design principle #2: maximize resolved shear stress for dislocation motion**
- **Design principle #3: dilute copper alloys are a good place to start**

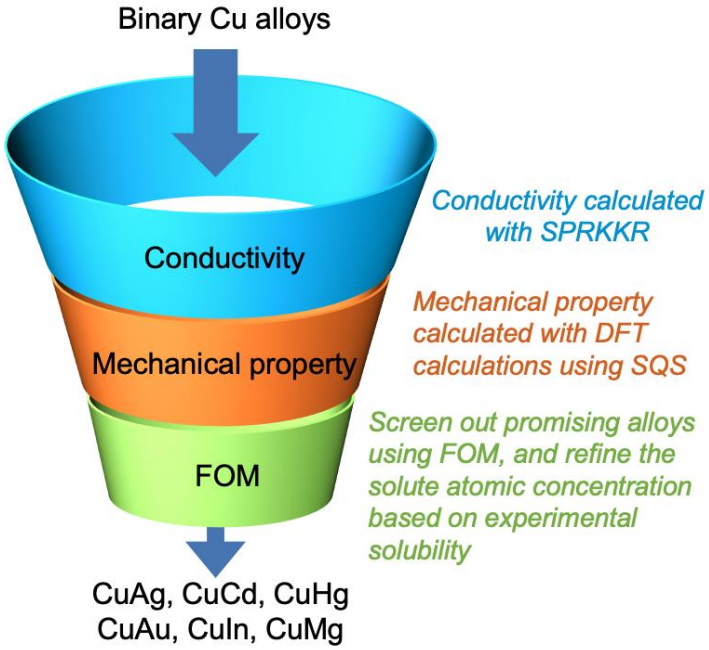
$$\mathrm{FOM} = \frac{\tau_{L-N}}{\varepsilon_{thermal}}$$

- Approach: high-throughput DFT calculations for dilute copper alloys

Wang, Simakov, Perez. *Applied Physics Letters* 120, no. 13 (2022): 134101.
Wang, Simakov, Perez. *Journal of Applied Physics* 132, no. 17 (2022).

Vignette #1.5: Can we design better materials?

- **Design principle #1: minimize RF losses**
- **Design principle #2: impede dislocation motion**
- **Design principle #3: dilute copper alloys are a good place to start**
- Approach: high-throughput DFT calculations for dilute copper alloys

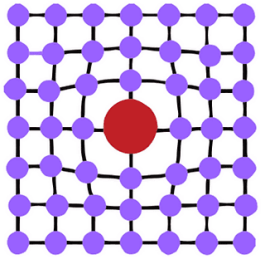


Wang, Simakov, Perez. *Applied Physics Letters* 120, no. 13 (2022): 134101.
Wang, Simakov, Perez. *Journal of Applied Physics* 132, no. 17 (2022).

FOM #1: Critical stress to move dislocations

Labusch–Nabarro (LN) model: Critical resolved shear stress required for dislocation motion:

$$\tau_{L-N} = \frac{(2\omega f_m^4 c^2)^{1/3}}{2b^{7/3}(Gb^2)^{1/3}}$$



With: $f_m = \frac{Gb^2}{120}\varepsilon_L$ $\varepsilon_L = \sqrt{{\varepsilon_G'}^2 + (\alpha\varepsilon_b)^2}$ $\left\{\begin{matrix} \alpha = 9-16 \\ \varepsilon_G' = \frac{\varepsilon_G}{1+0.5|\varepsilon_G|} \end{matrix}\right\}$

Two key parameters:

- Size misfit $\varepsilon_b = \frac{db}{bdc}$
- Modulus misfit $\varepsilon_G = \frac{dG}{Gdc}$

Zander et al., Computational Materials Science 41 (2007) 86–95
Butt, Journal of Materials Science 28 (1993) 2557-2576

FOM #2: Thermal stress created by RF dissipation

- Assuming that the surface is free to relax in z only, the corresponding in-plane thermal stress is

$$\varepsilon_{xx} \equiv \varepsilon_{yy} \equiv -\frac{E\alpha\Delta T}{1-v}$$

- Heating due to RF losses can be estimated from the solution of the heat equation:

Accelerator parameters $\Delta T = \frac{G^2\sqrt{T_p}}{Z_H^2}\frac{R_s}{\sqrt{\pi\rho c_\varepsilon k}}$ Material properties

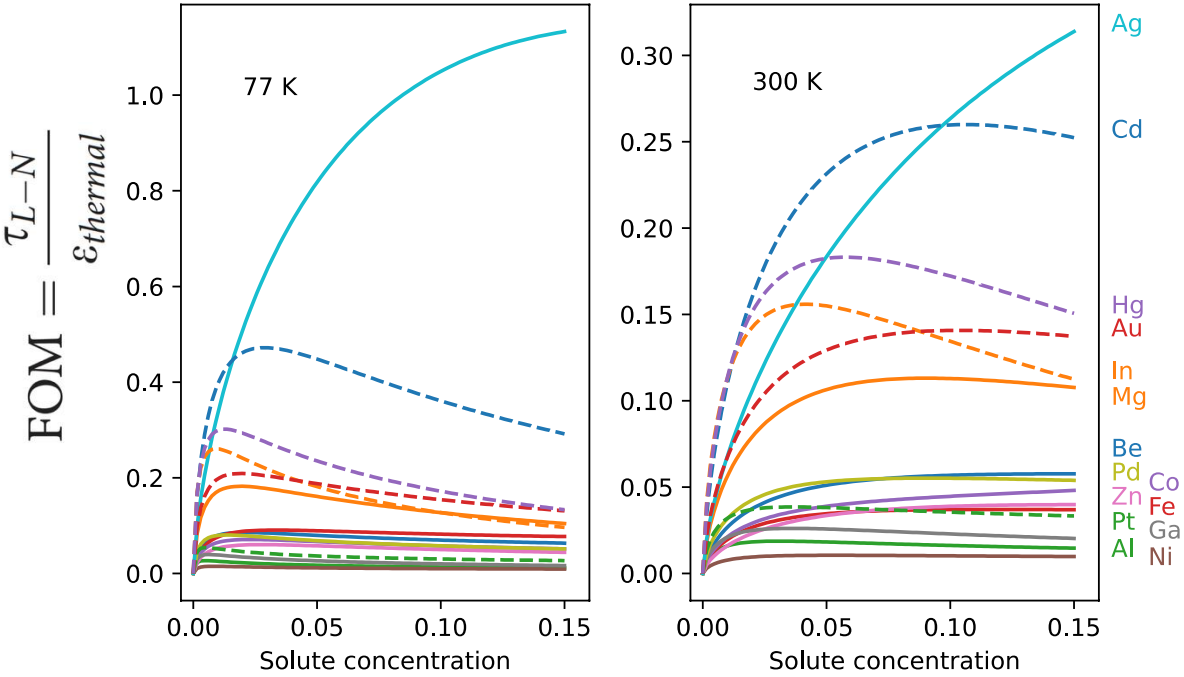
TABLE I. Parameters of a sample C-band accelerating structure.

Parameters	λ	T_p	G	Z_H
Values	0.052 m	1.0 μs	100 MV/m	$\frac{Z_0}{1.25} = \frac{377\,\Omega}{1.25} = 301.6\,\Omega$

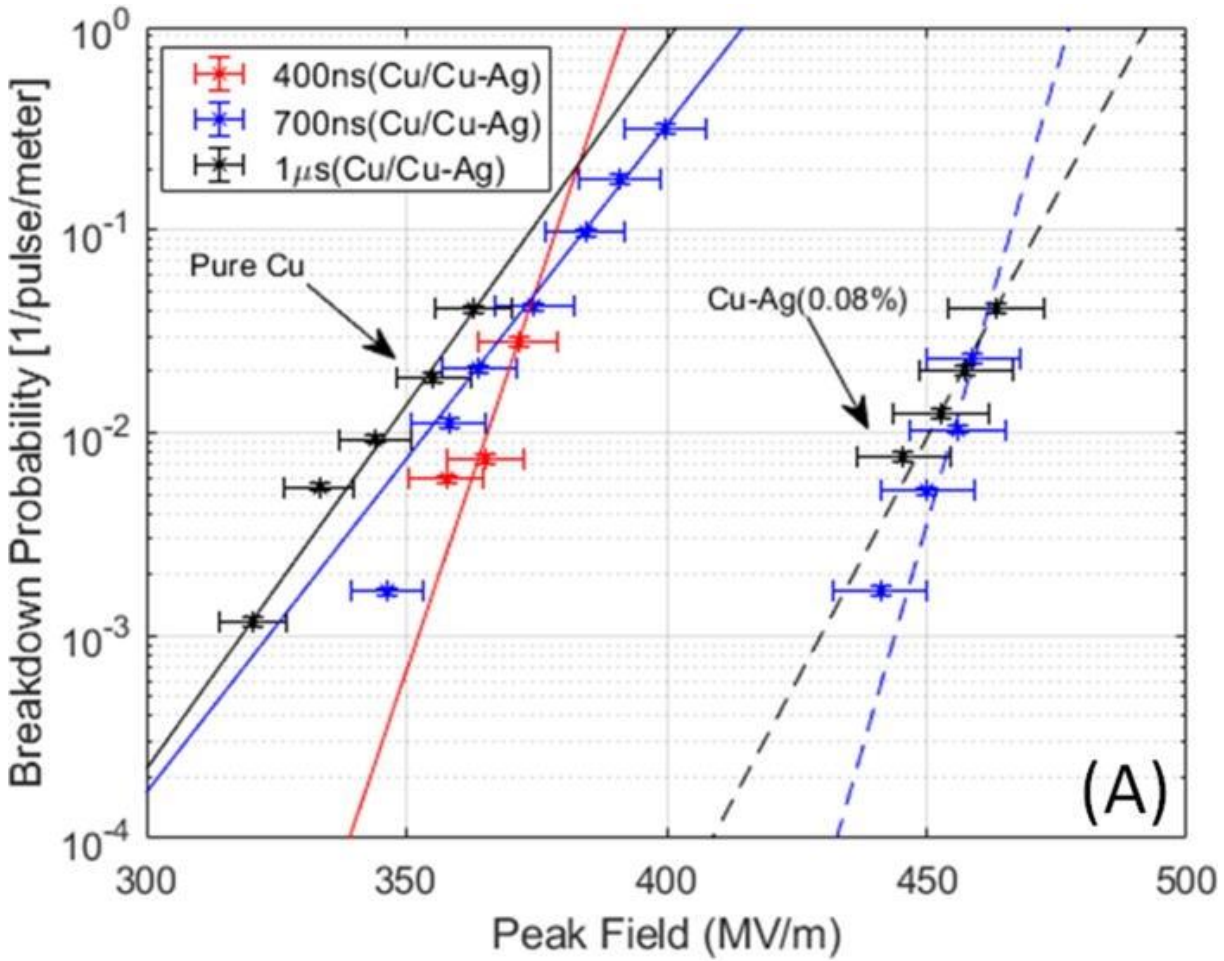
Perry B. Wilson. In ITP Conference on Future High Energy Colliders. University of California, Santa Barbara, October 1996.

Alloy design

Ag, Cd, Hg, Au, In, and Mg stand out as potential alloying candidates.



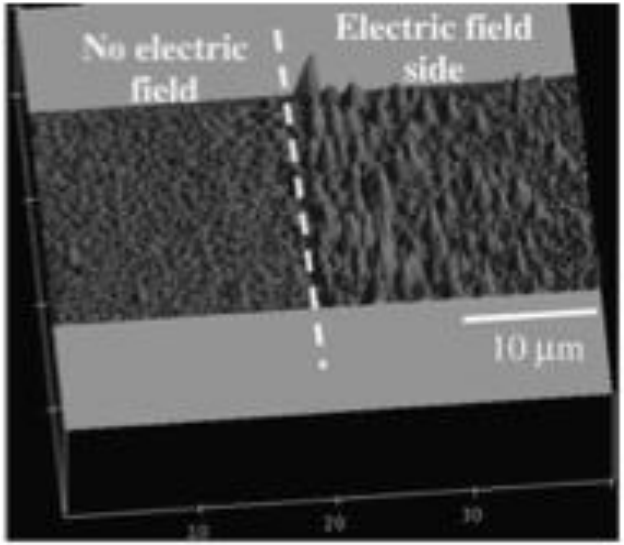
- **Ag, Cd:** excellent conductivity
- **Hg, In, Cd**: strong strengthening
- **Au, Mg**: decent at both



Schneider, et al. *Applied physics letters* 121.25 (2022)

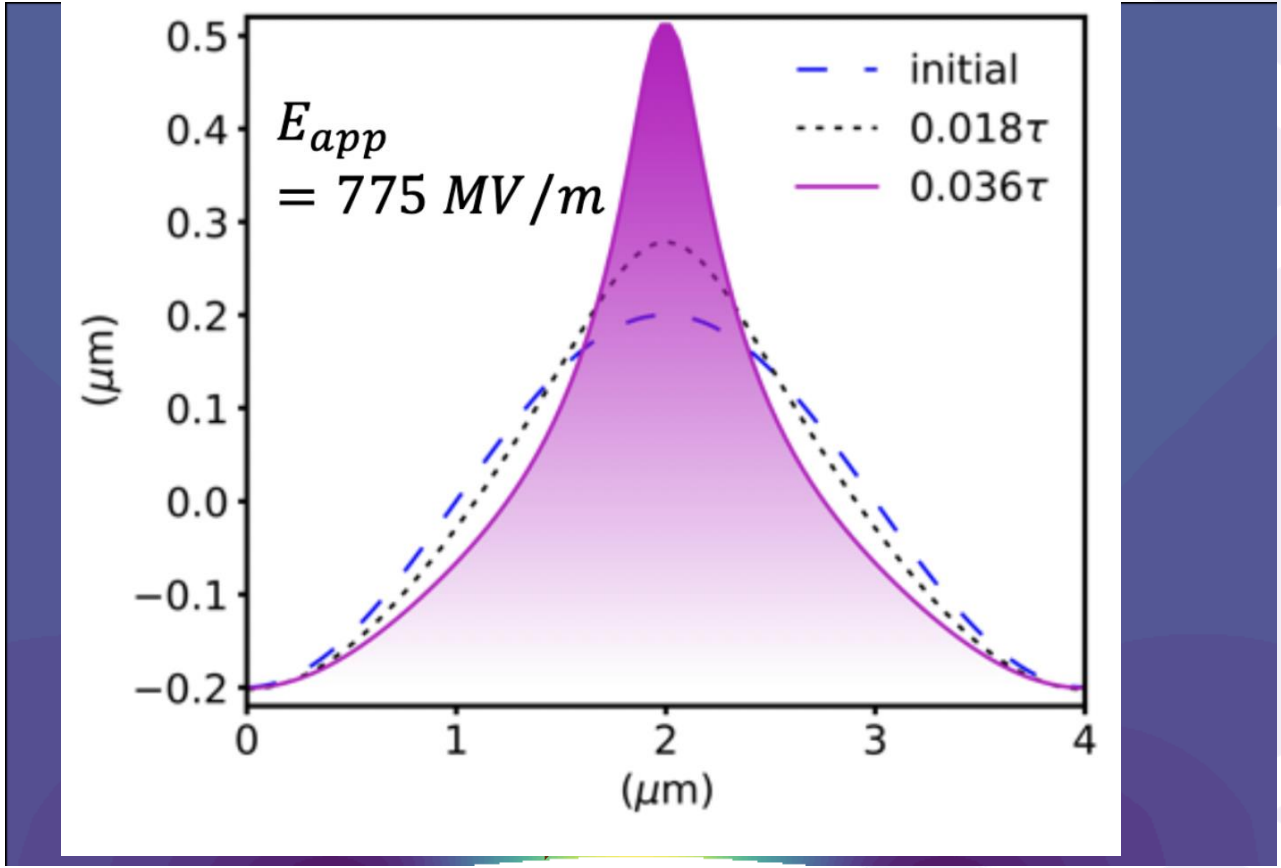
Vignette #2: Surface-transport induced roughening

- Surface roughening also occurs without thermo-elastic stress, e.g., under DC electric fields
- Suggests that another mass transport mechanism operates
- Prime suspect: **surface diffusion**

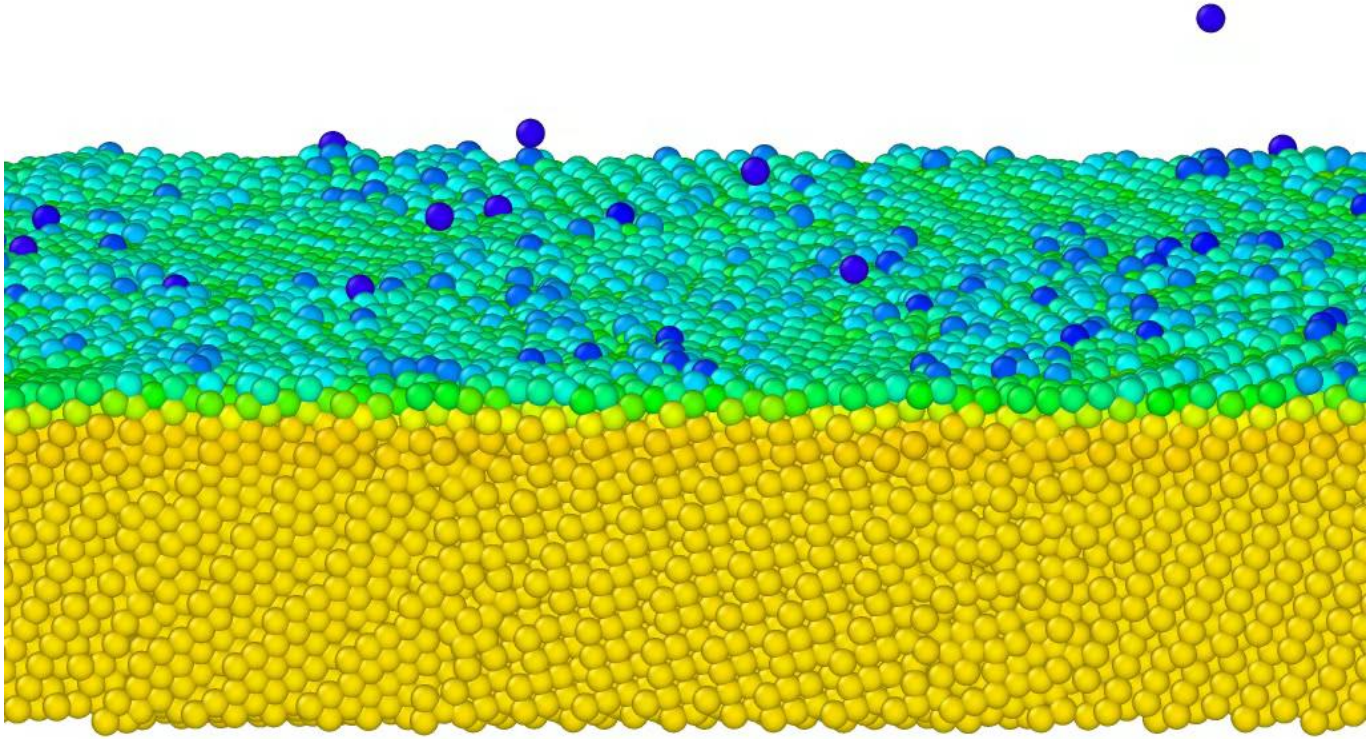


[Gill, Goduru, Sheldon (2008)]

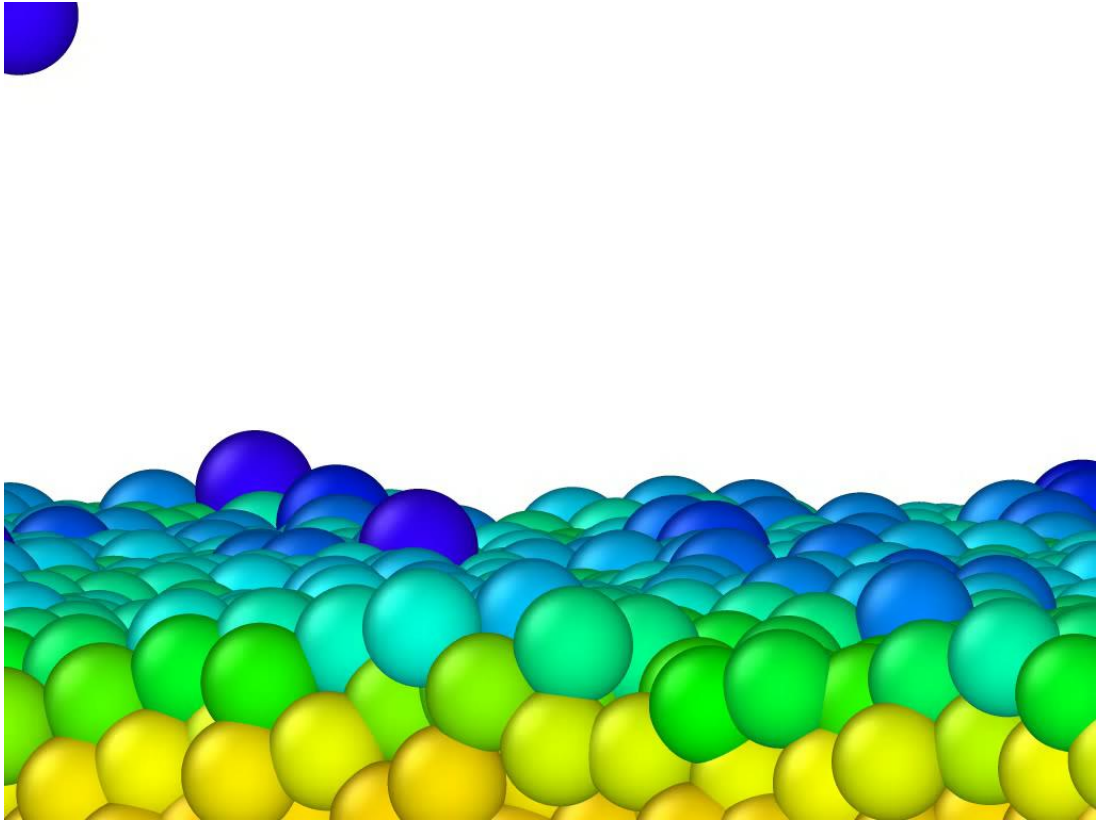
Physical intuition: field



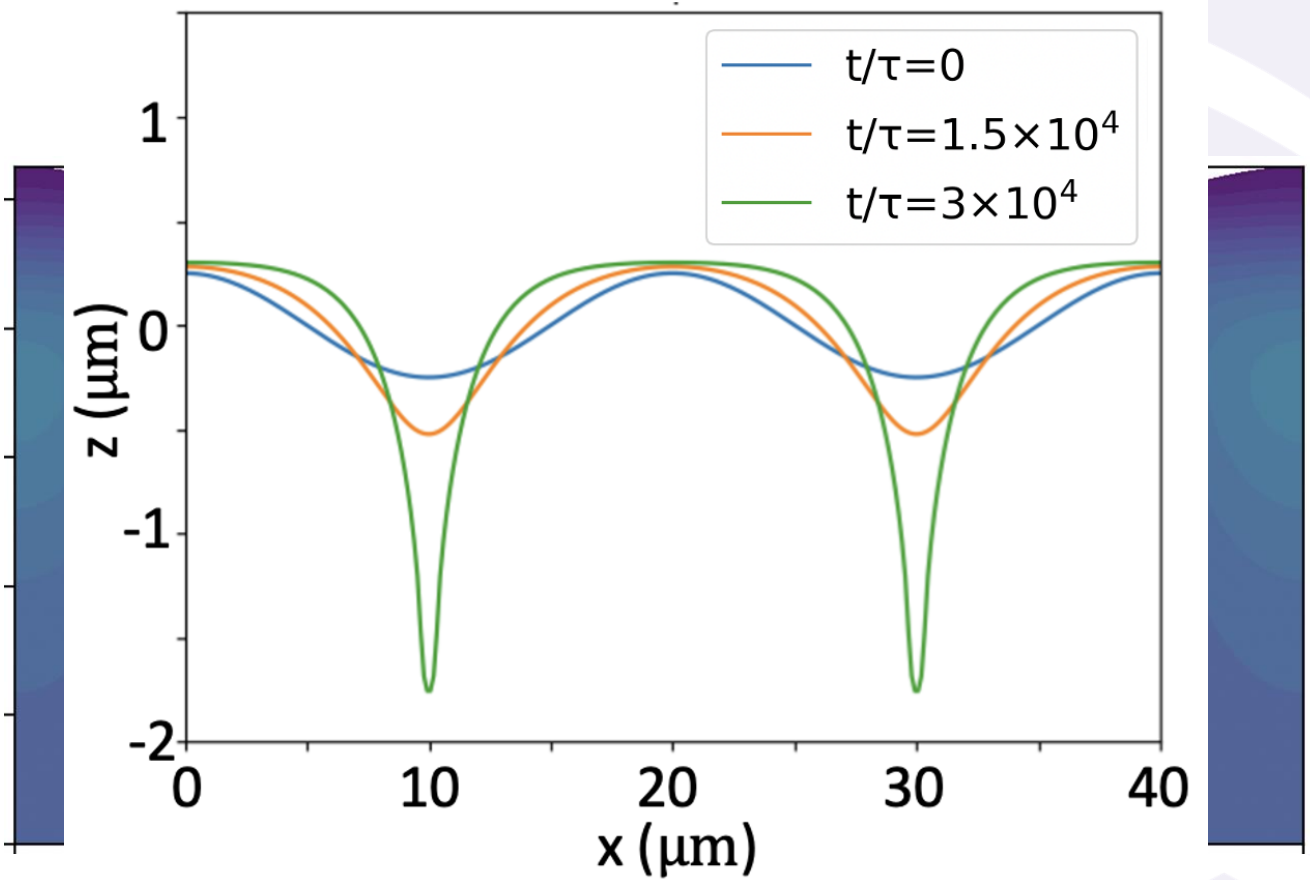
Direct atomistic simulations



Direct atomistic simulations



Physical intuition: thermo-elasticity



Linear stability analysis

Driving forces:

- Surface tension
- Electrostatic energy
- Thermo-elastic stresses

Dynamics:

- Surface diffusion along chemical potential gradient

Under an applied field **E** and a stress caused by a temperature rise **ΔT**, the amplitude of a mode of wavenumber **k** grows as:

$$h(t,k) = h_0(k)\exp\left(C\left(2k^3\alpha^2\boldsymbol{\Delta T^2} + k^3\epsilon_0\boldsymbol{E^2} - \gamma k^4\right)t\right)$$

Thermoelastic stresses ↑ E-field ↑ Surface tension ↓

[Shinohara, Bagchi, Simakov, Baryshev, Perez (2024); Song, Yang (2006); Du, Srolovitz (2004)]

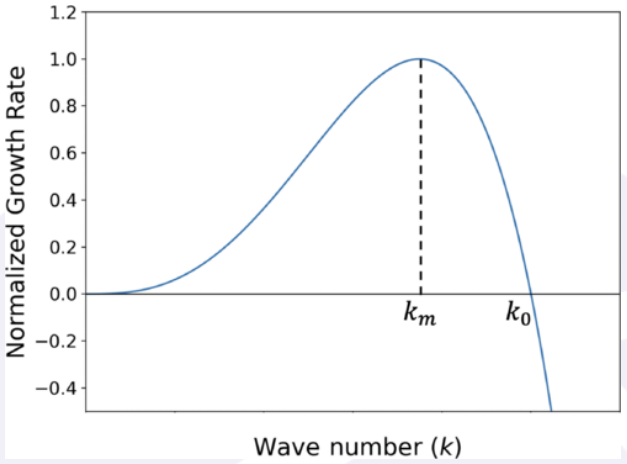
Linear stability analysis

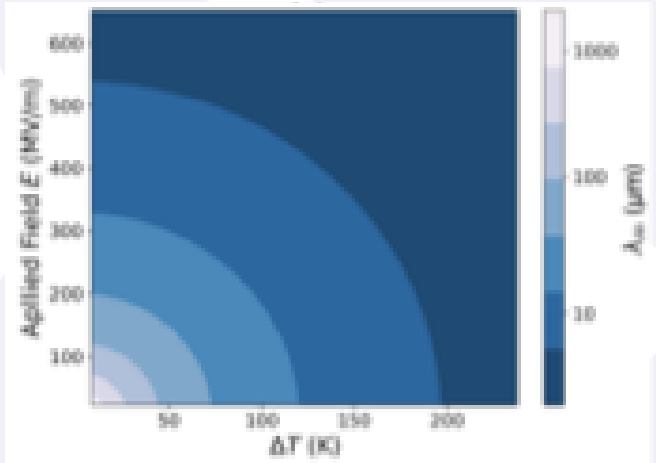
- Growth rate of the maximally-unstable mode is very sensitive to E and ΔT

$$h(t,k) \sim \exp\left(-\frac{E_b}{k_B(T+\Delta T)}\right)[E^2+\Delta T^2]^4$$

- **Very sharp dependence on E and ΔT**

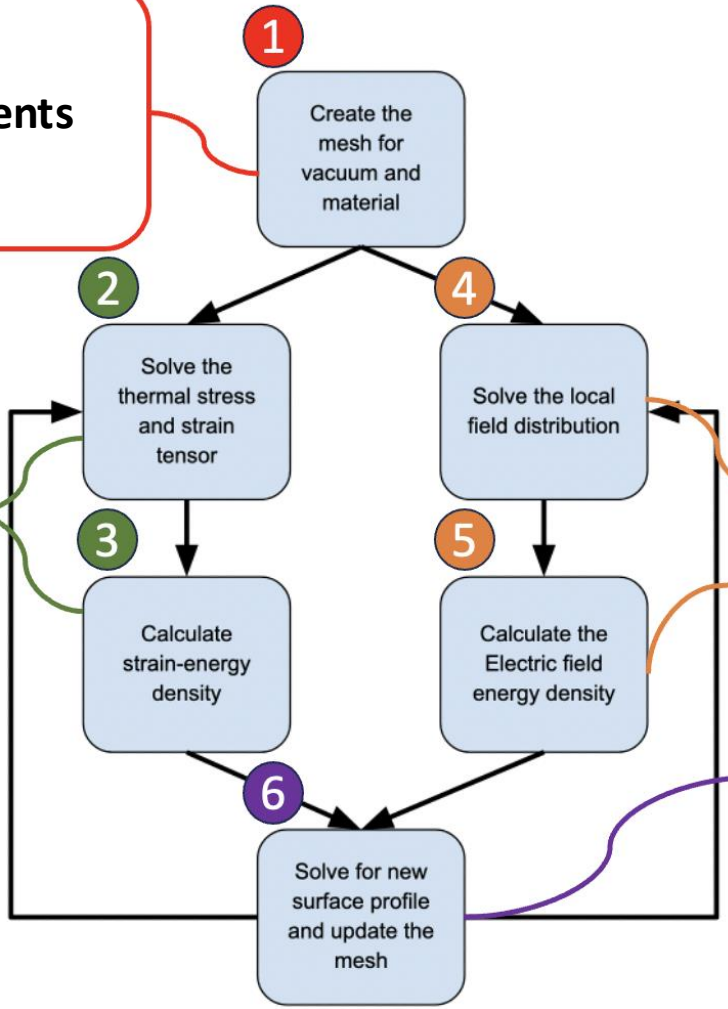
- Non-linearities and finite amplitudes further increase coupling





[Shinohara, Bagchi, Simakov, Baryshev, Perez (2024)]

Method: 2D finite elements



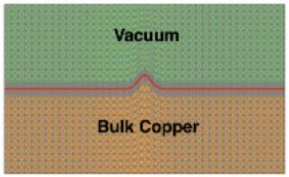
Driving force #1: Electrostatics of field-induced charges

Driving force #2: Thermo-elasticity induced by resistive heating

Surface diffusion along chemical potential gradient

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

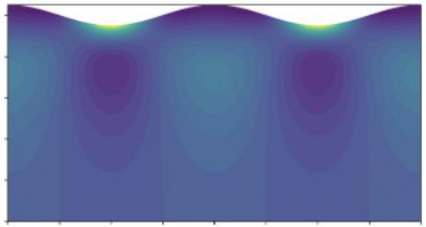
$$-\nabla \cdot \sigma(u) = 0$$

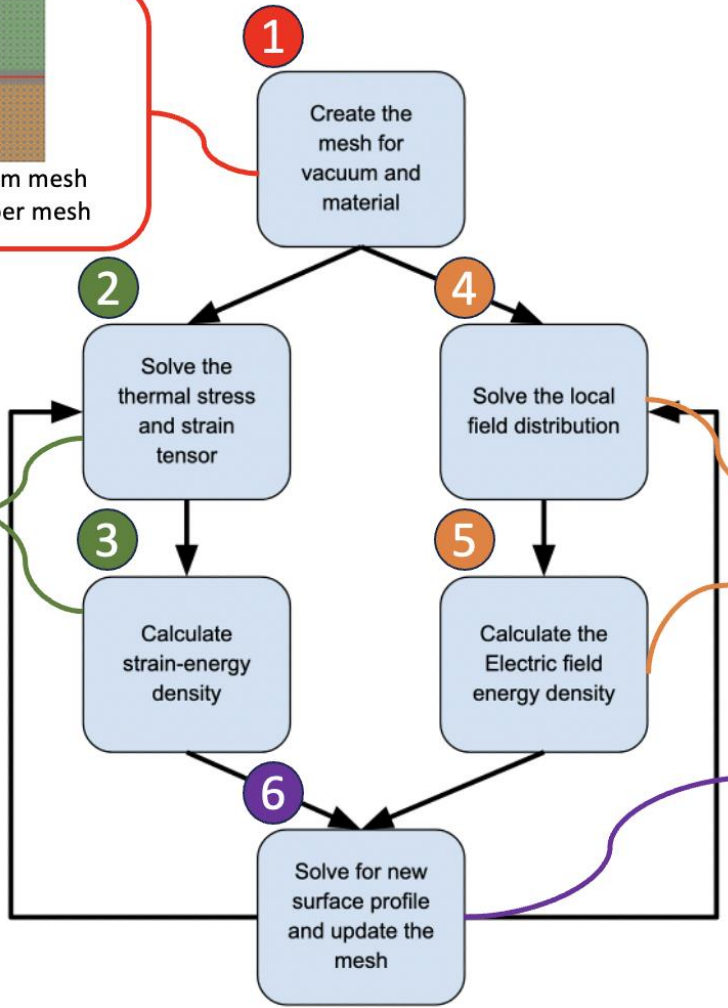
$$\sigma(u) = \lambda tr(\epsilon(u))\mathbb{1} + 2\mu\epsilon(u) - \frac{\alpha Y}{1-2\nu}\Delta T\mathbb{1}$$

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

Strain-Energy Density

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





4 & 5

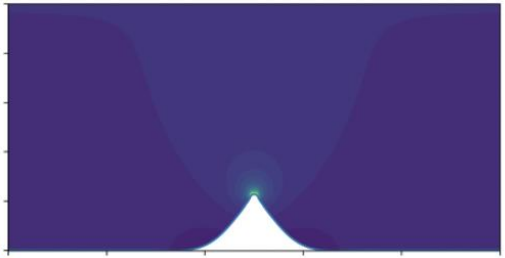
Electrostatic

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

$$E = -\nabla\phi$$

Field Energy Density

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



6

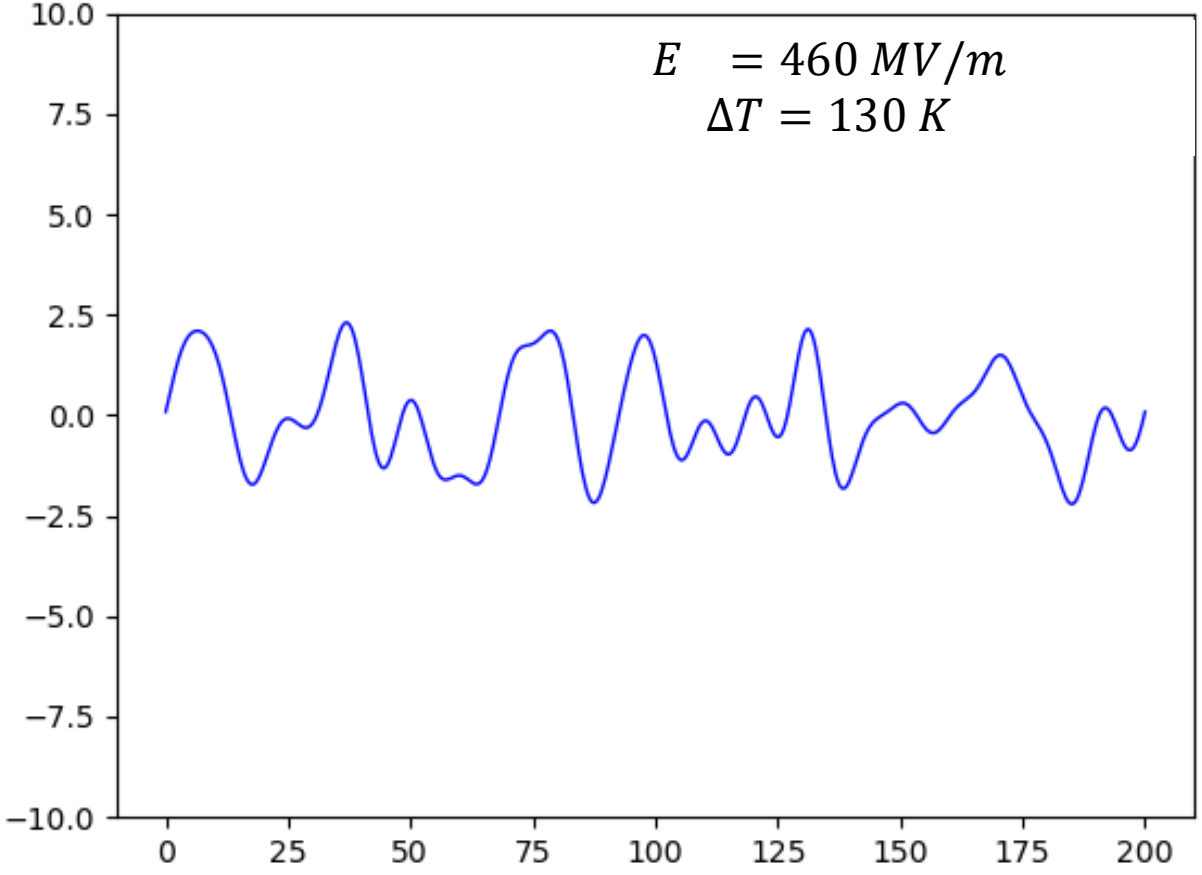
Surface Diffusion

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

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

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

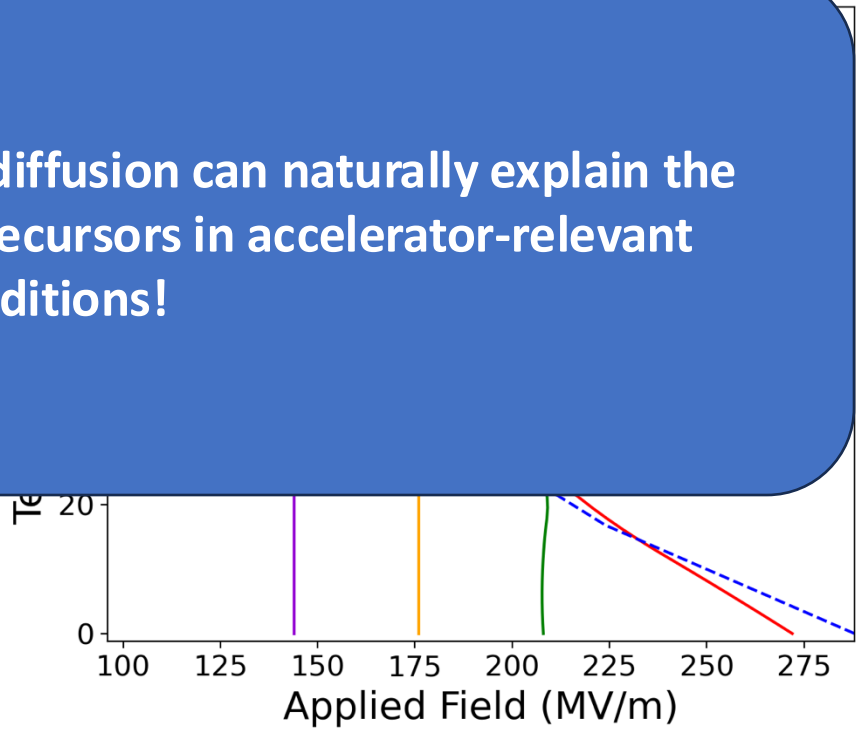
Chemical potential = surface tension + electrostatic energy + strain energy density


$E = 460\ MV/m$
$\Delta T = 130\ K$
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
0
25
50
75
100
125
150
175
200

Tip runaway phase diagram

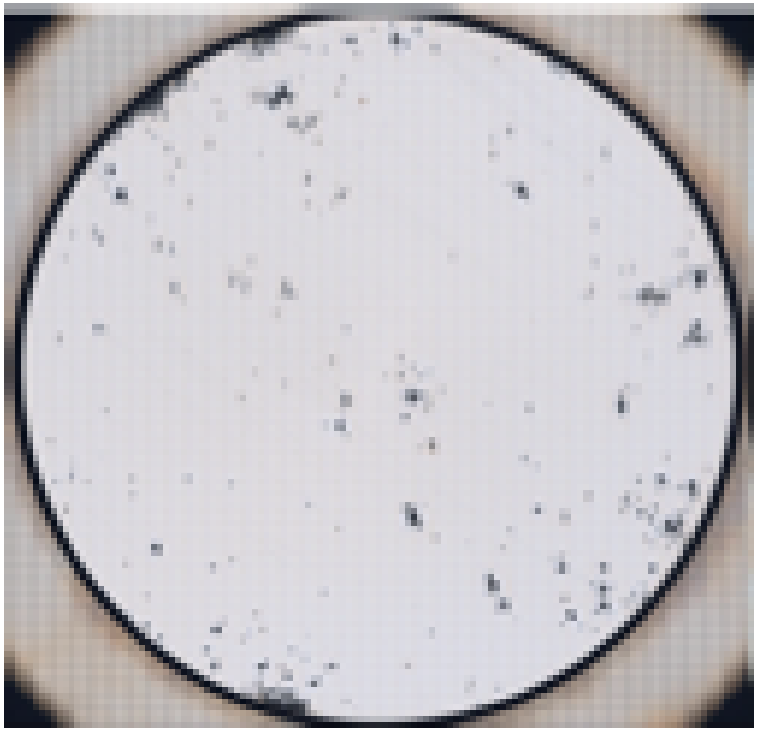
- **Nominal surface features:**
  - Th
    lo
  - To
    ar
- **Sha**
  - E
  - R
- **Cor**
  - **precursor formation around O(100-200) MV/m**
  - **increased breakdown with cyclic heating**
  - **secondary breakdowns**

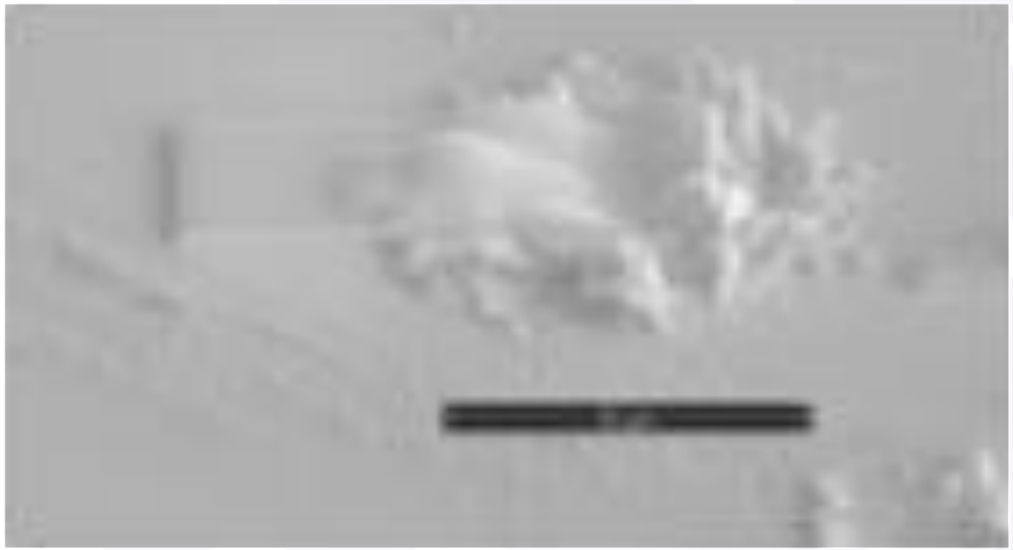
Roughening through surface diffusion can naturally explain the formation of breakdown precursors in accelerator-relevant conditions!



[Shinohara, Bagchi, Simakov, Baryshev, Perez (2024)]

Most breakdown events are “secondary”





[Wuensch et al, arXiv:2502.03967]

Summary

- Breakdown likely originates from multiple synergistic and competing factors

- In “standard” room temperature RF operation, it is plausible that:
  - Thermoelastic effects such create initial roughness
  - Field-driven surface diffusion sharpens precursors
  - For near-critical precursors, field-enhanced plasticity also activates
  - Previous breakdown sites act as likely nucleation sites for further breakdown

- The kinetic competition between the different modes needs to be better understood

- Other factors are likely to be important: oxide layers, contaminant molecules, impurities,… More work required.

Acknowledgements

- **Soumendu Bagchi:** MD simulations, FEM modeling
- **Ryo Shinohara:** FEM modeling, generalization to semi-conductors
- **Gaoxue Wang:** Materials Design

Funding:

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT