Atomistic modeling of the coupling between electric fields and bulk plastic deformation in RF structures

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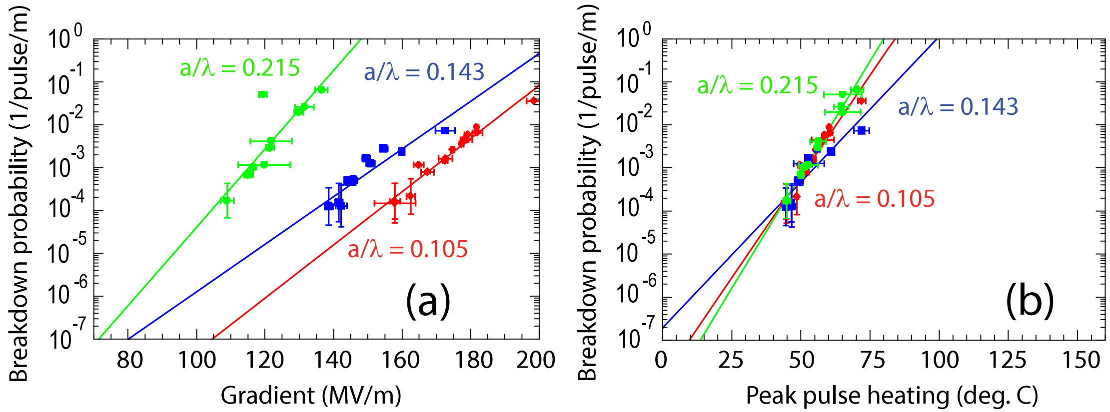
Motivating challenges

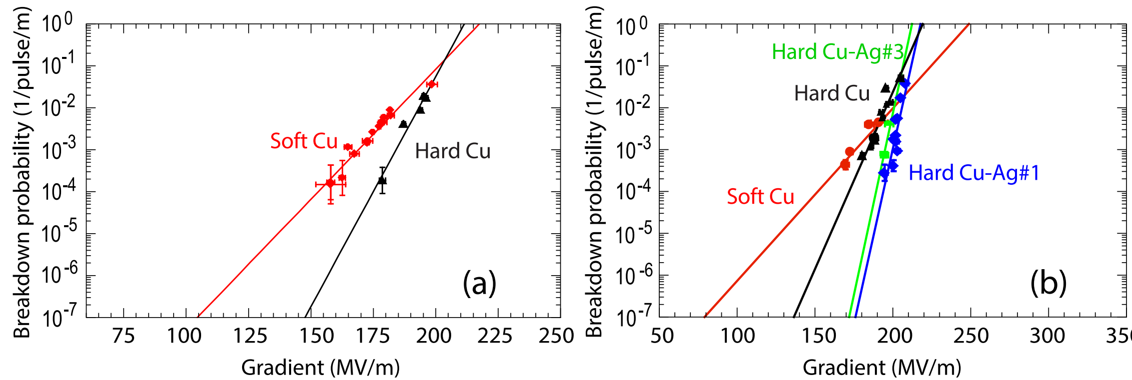
- Compact, low-cost, accelerators require high gradients
- Increase in gradients limited by RF breakdown
- Incidence of breakdown is very well characterized (SLAC, CERN, KEK, INFN-LNF, etc.)
- Microscopic causes are complex:
  - occurs at fields that are well below what needed of a clean flat Cu surface (~10 GV/m)
  - implies the formation of surface precursors that locally enhance the field

Motivating questions

- What are these precursors and how they form?
- What controls their formation rate?
  - Gradients
  - Peak pulse heating
  - Chemical composition
  - Bulk microstructure
  - ???



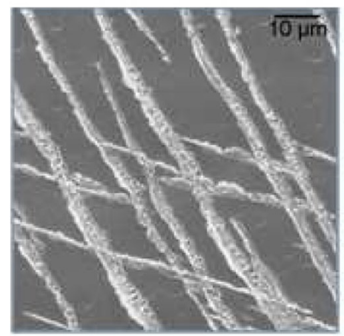
Dolgashev, Tantawi, Higashi, Spataro, 2010

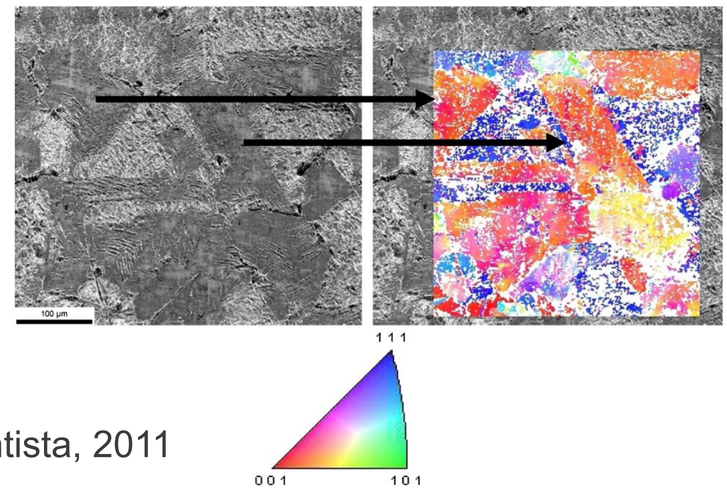


Simakov, Dolgashev, Tantawi, 2018

Background

Strong indications that thermal fatigue plays a key role



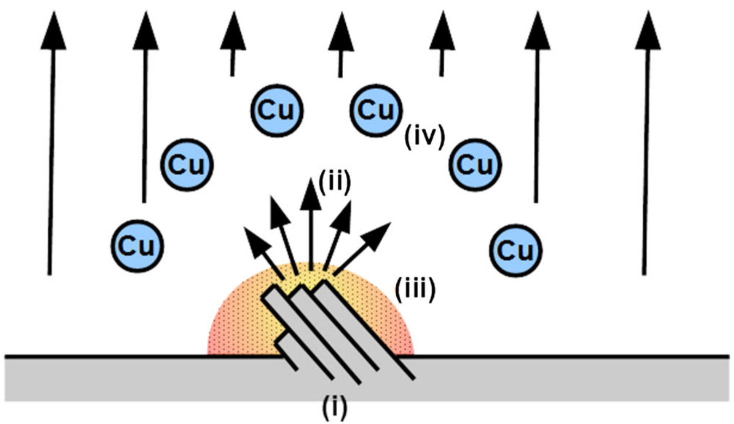


Laurent, Tantawi, Dolgashev, Nantista, 2011

This mechanism couples to composition/microstructure

Background

In fatigue, surface deformation is mediated by dislocations incoming from the bulk



Engelberg et al, 2019

- Plastic deformation in real materials is **extremely** complex
- Heroic efforts to model evolution of dislocation distribution under field [e.g., MDDF by Ashkenazy et al.]
- Important takeaway: key parameter is β, which relates applied E to resolved shear stress

Our approach

- **Goal:** *begin* to understand the *coupling between the surface tractions induced by E and plastic deformation*

- **Idealized** setting

- Main tool: Atomistic level modeling using Molecular Dynamics

Summary of today's talk:

- Atomistic charge equilibration model
- Plastic deformation under E field

Levels of theory

Quantum description:

– Density functional theory (DFT)

- Strengths:
  – Very accurate
  – Natural description of E
- Weakness:
  – Very expensive (scales as $N_{electrons}^3$)
    - Small systems (~few 100 atoms):
    - Static or short dynamic simulations (~ps)

Classical description:

– Molecular dynamics

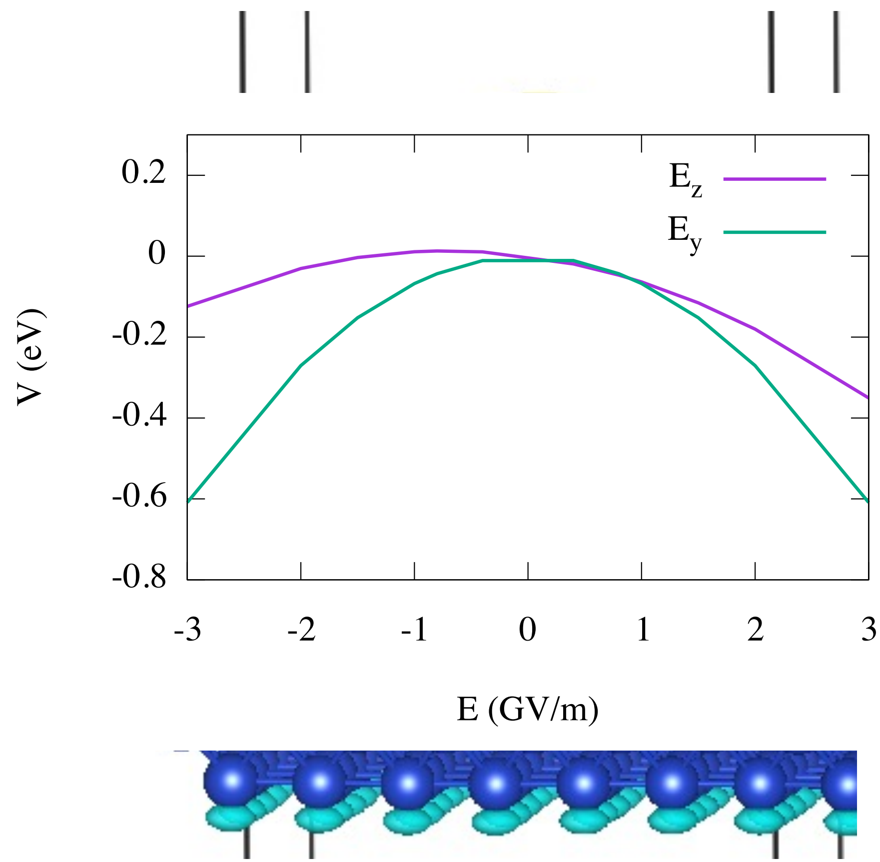
- Strengths:
  – Relatively fast
    - "Large" systems (>10^6 atoms)
    - "Long" simulations (10^{-6}-10^{-3} s):
- Weakness:
  – E has to be included "by hand"
  – still << engineering scales

Classical MD

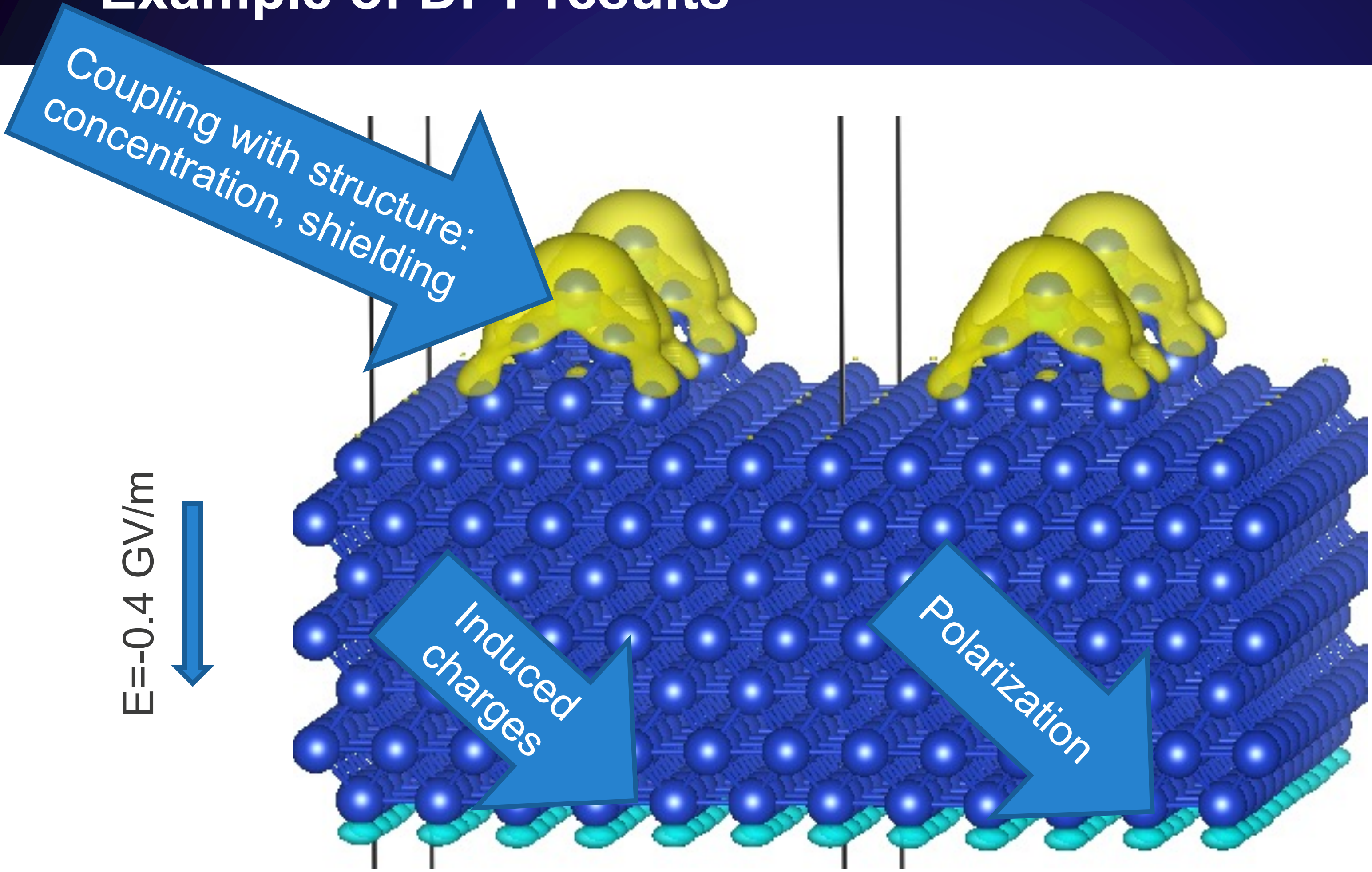
In conventional MD, charges are typically implicit or fixed. In order to capture field effects, we need a **charge equilibration model.**

1. Parameterize the empirical electronic Hamiltonian by fitting to quantum data

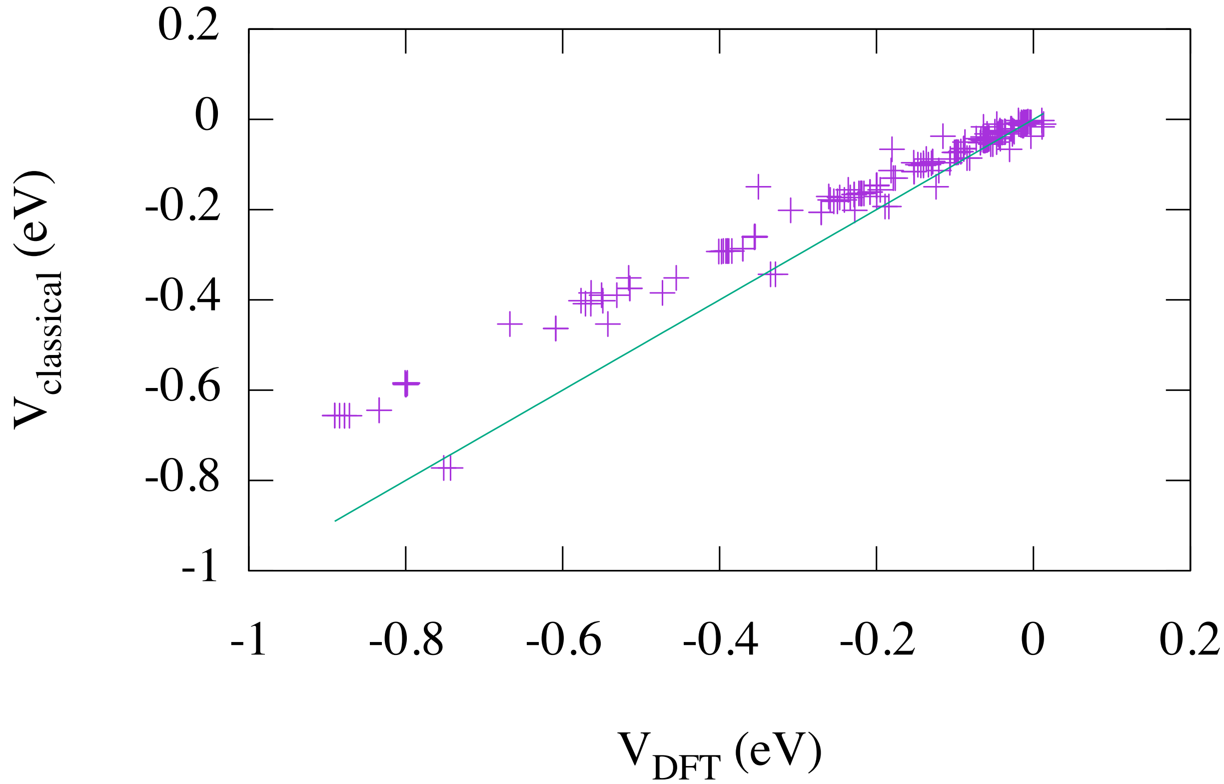
2. During MD: dynamically assign charges to minimize electronic energy



Example of DFT results



Validation: no polarizability, no intrinsic dipole



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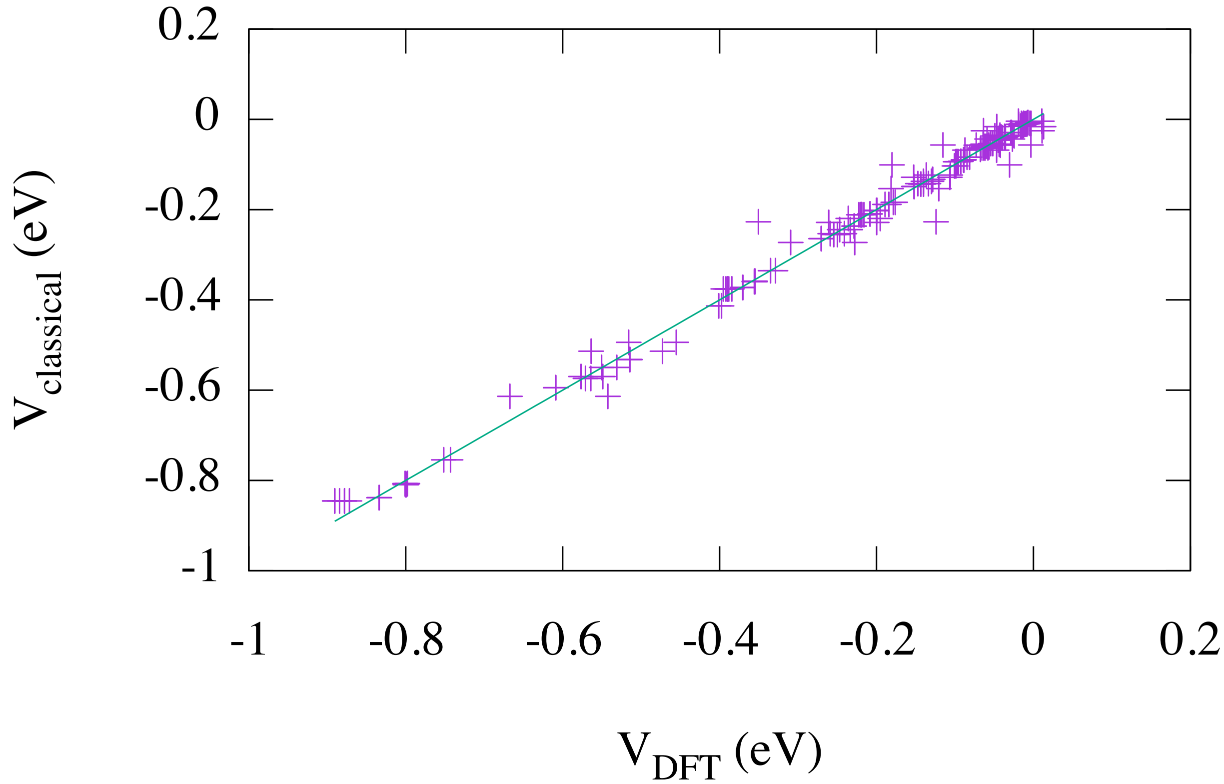
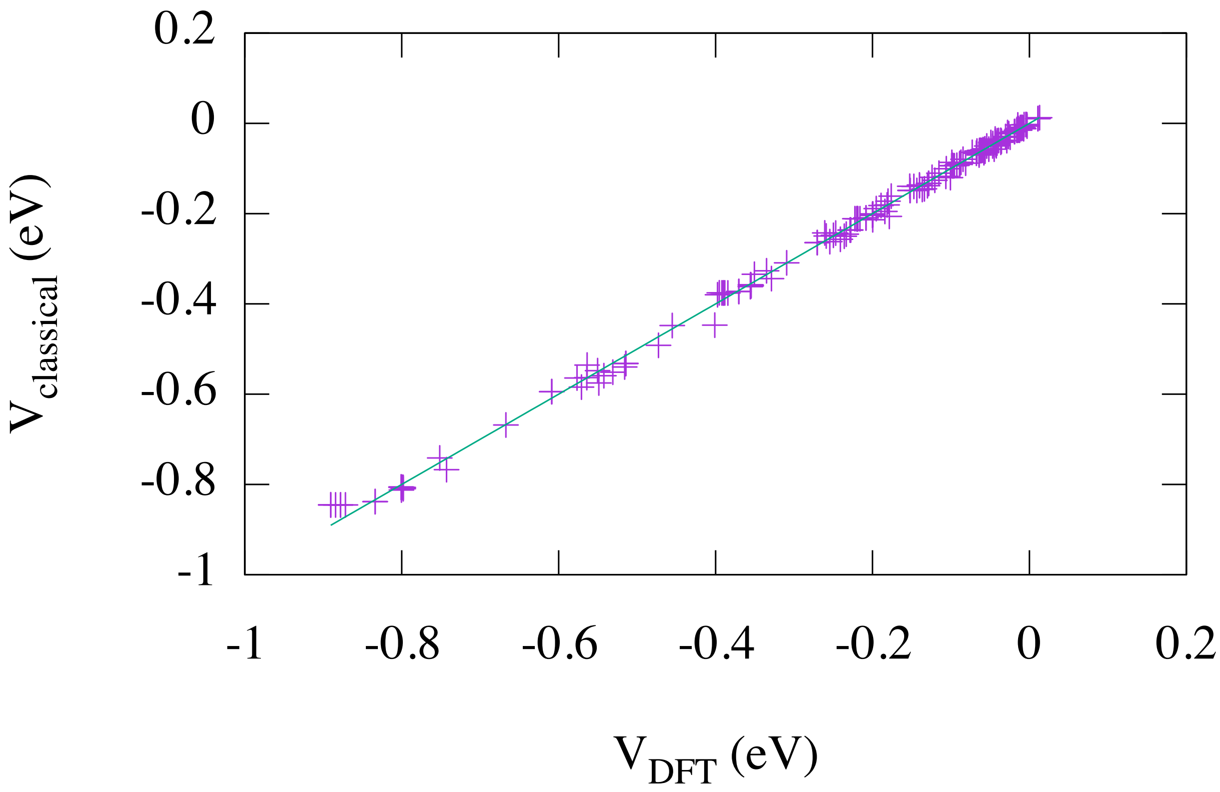
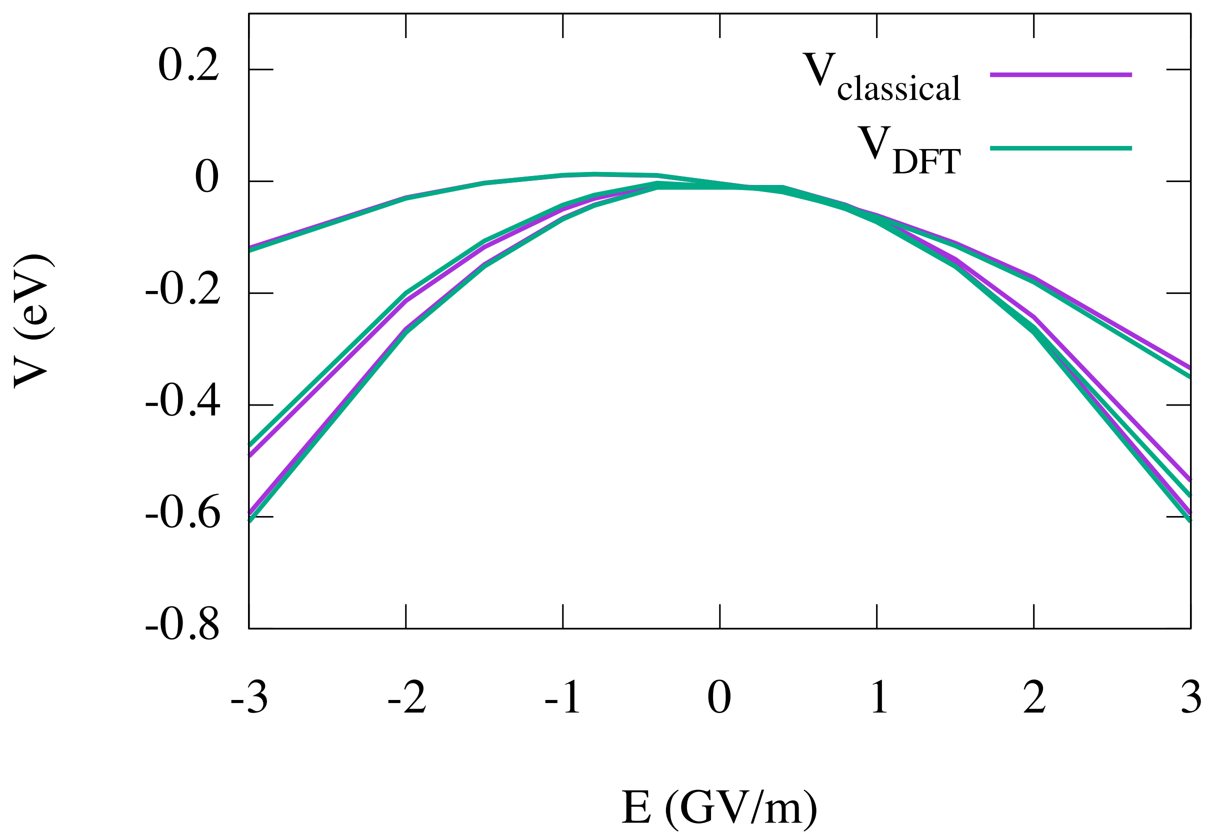


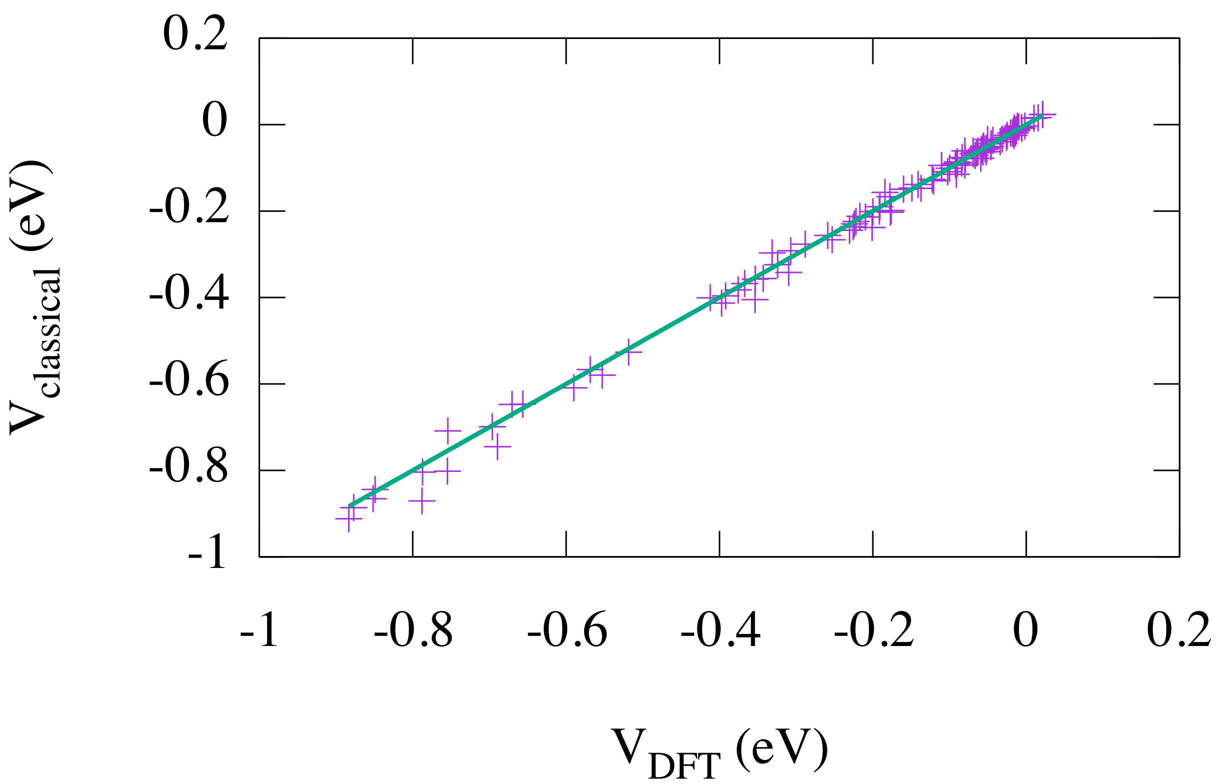
Validation: polarizability, intrinsic dipole



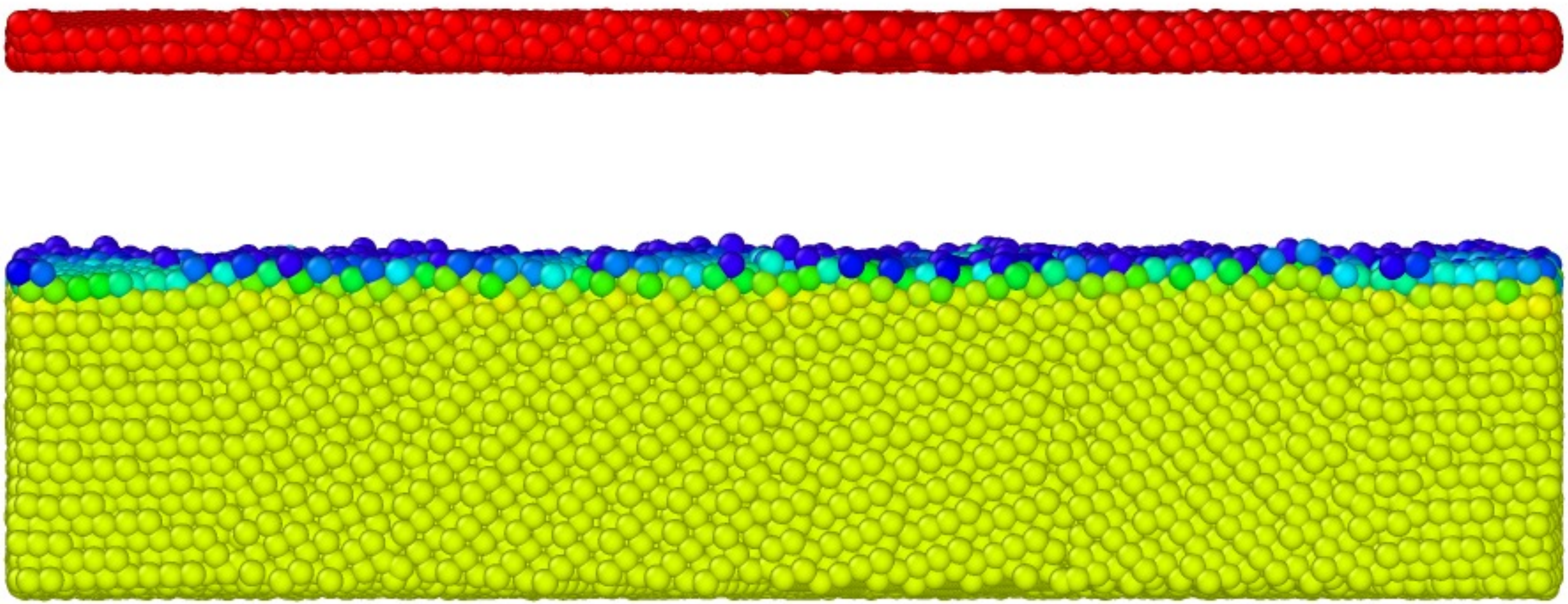
Intrinsic dipole



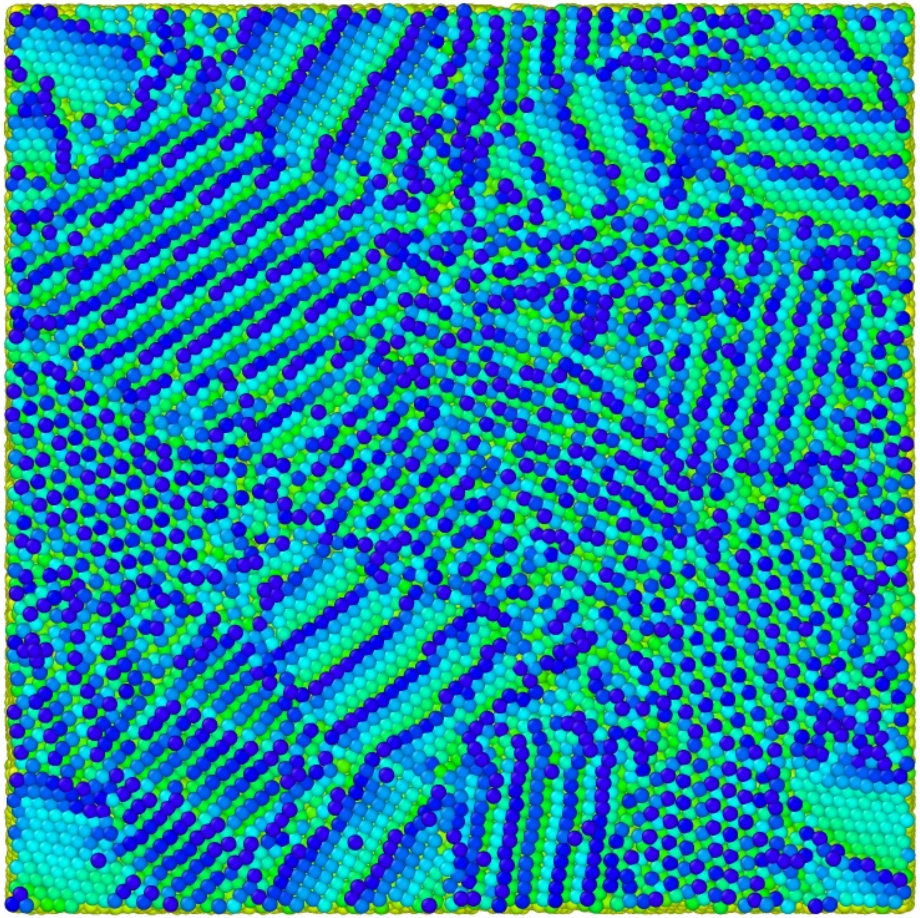
Validation Cu/Ag: polarizability, intrinsic dipole



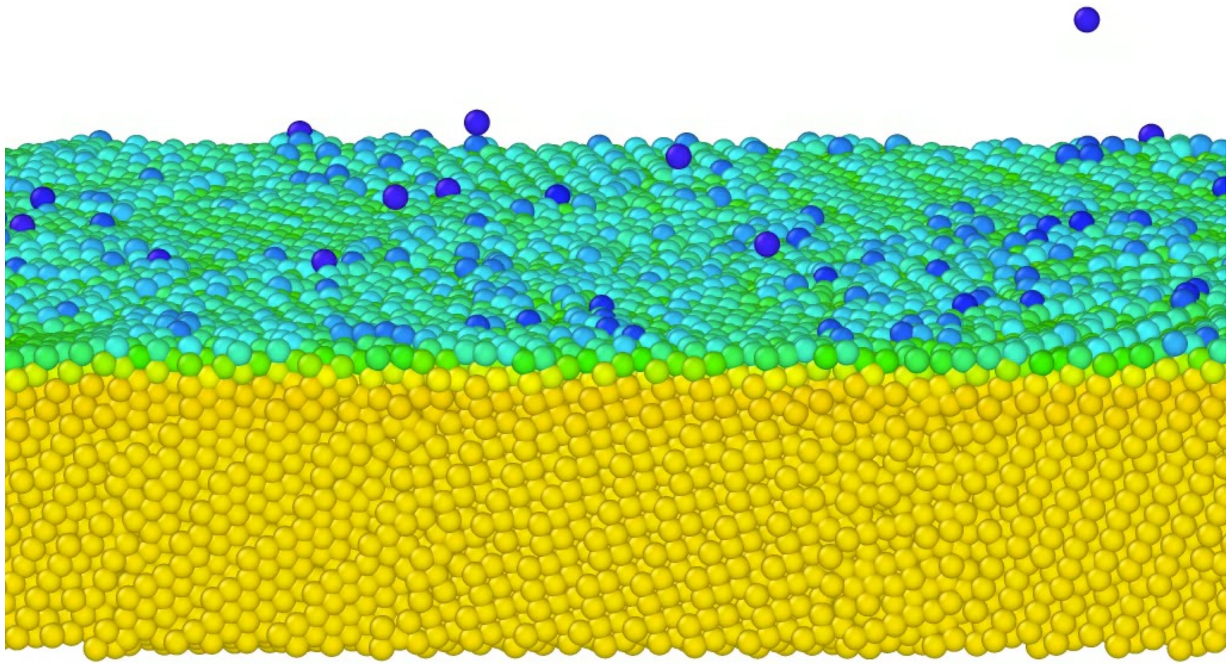
Model #1: Large-scale MD



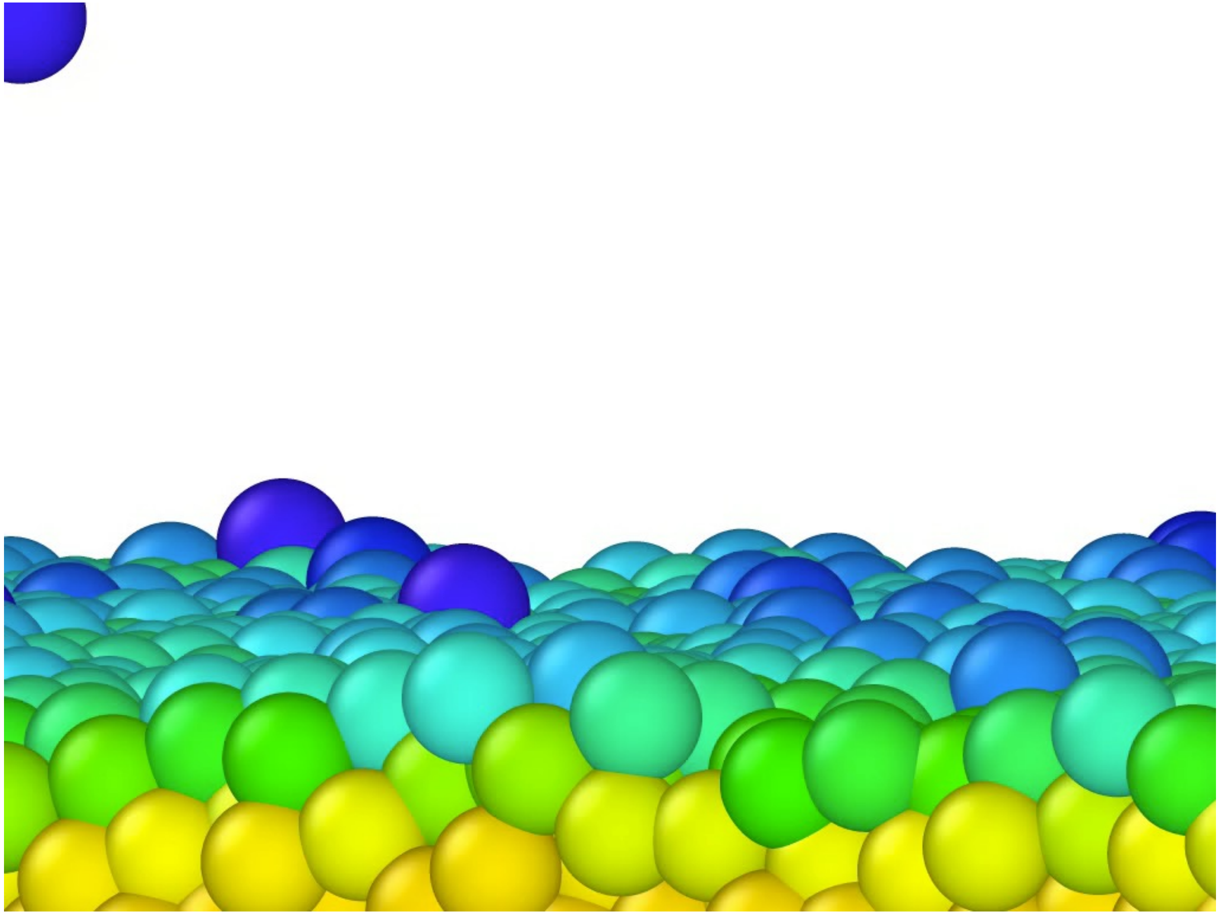
Large-scale MD



Large-scale MD

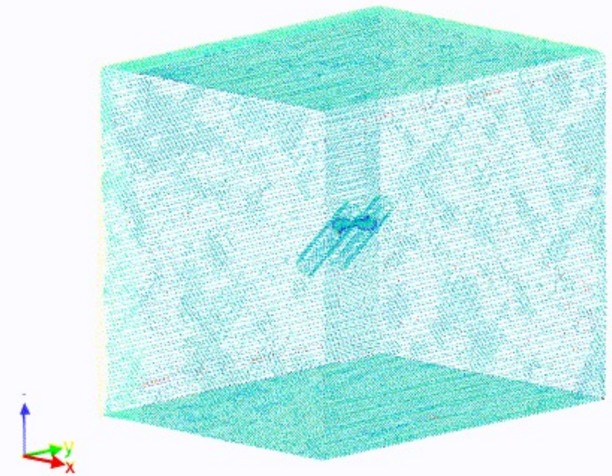


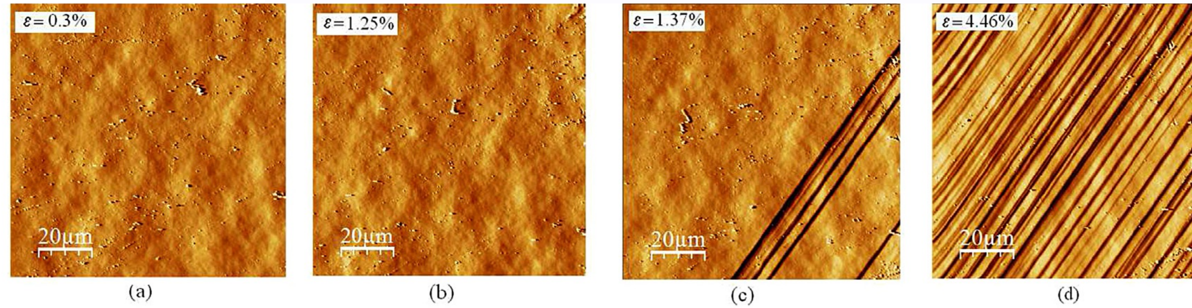
Large-scale MD



Plastic deformation under E

- Fully-developed dislocation microstructure is incredibly complex
- Considering unit steps in isolation
- **First target: 1D periodic array of Frank Read sources**

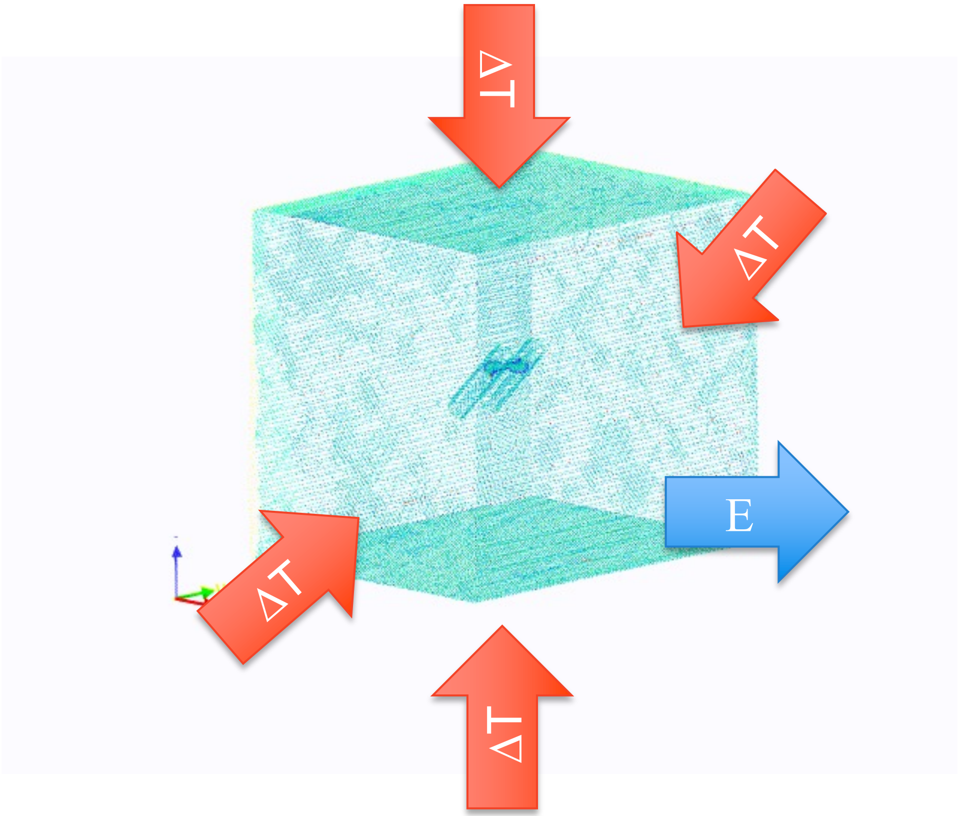




Setup

Driving forces:

- Lateral thermal stress due to RF heating
- Surface traction due to field-induced surface charges

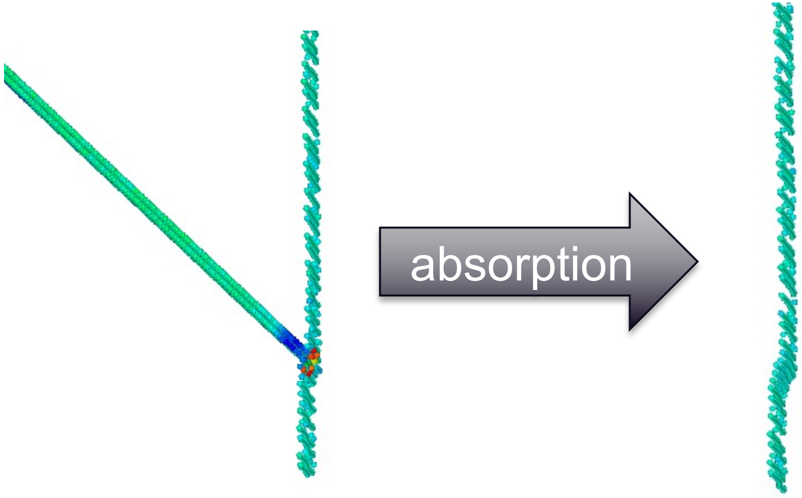


Setup

Driving forces:

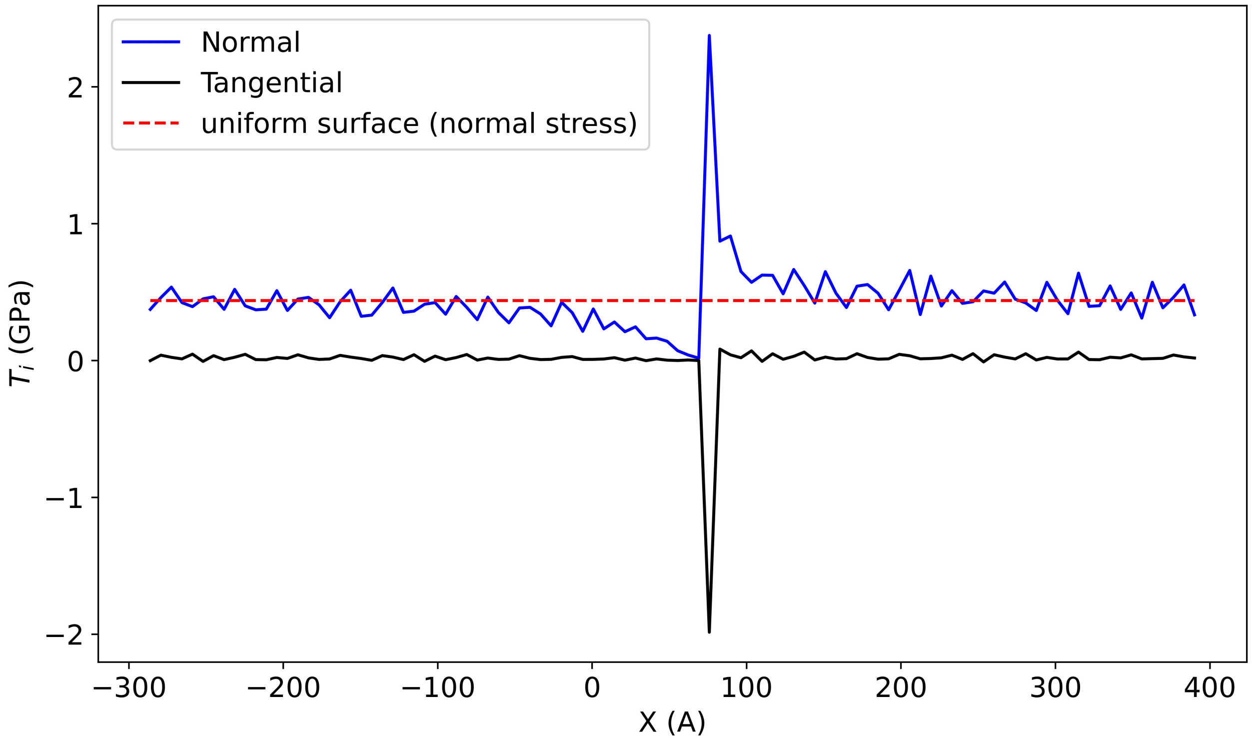
- Lateral thermal stress due to RF heating
- Surface traction due to induced surface charges

- Field enhancement due surface steps (MD-QEq)

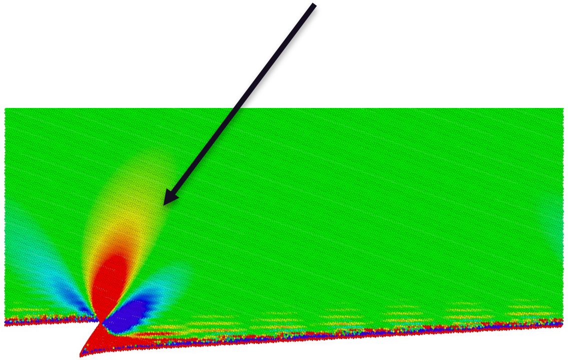


RSS enhancement due to surface steps

10 GV/m



Asymptotic decay ~ 1/r



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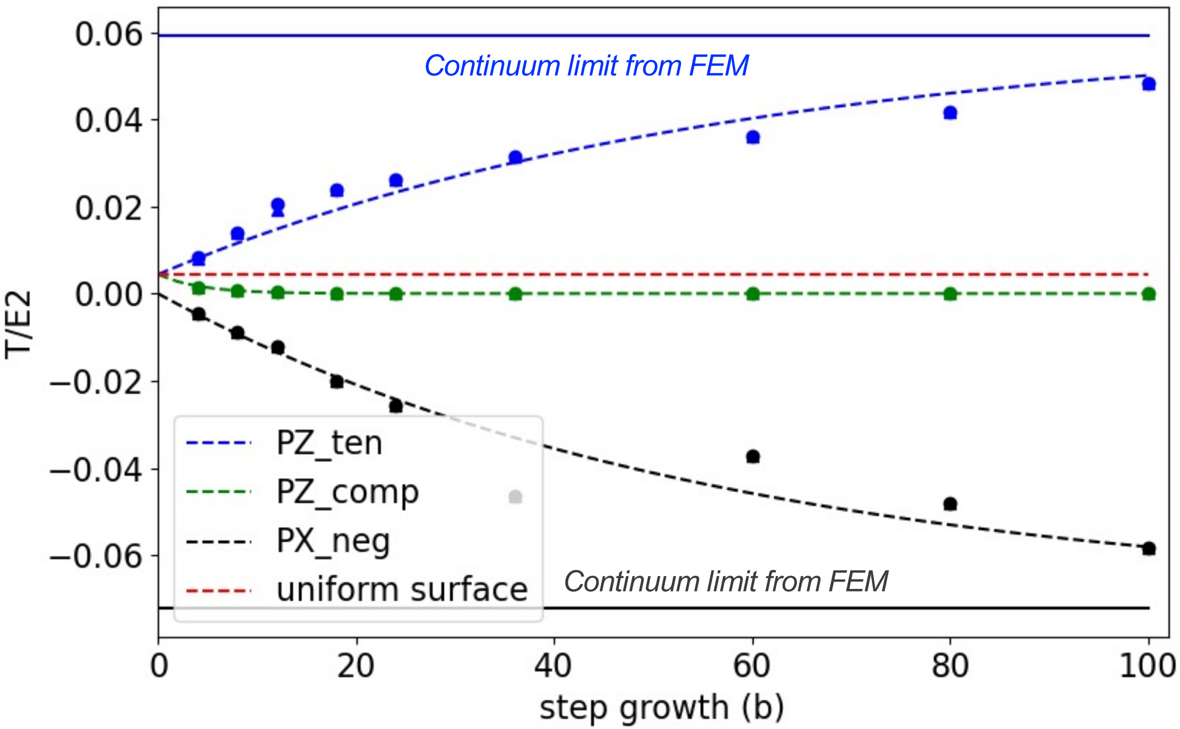
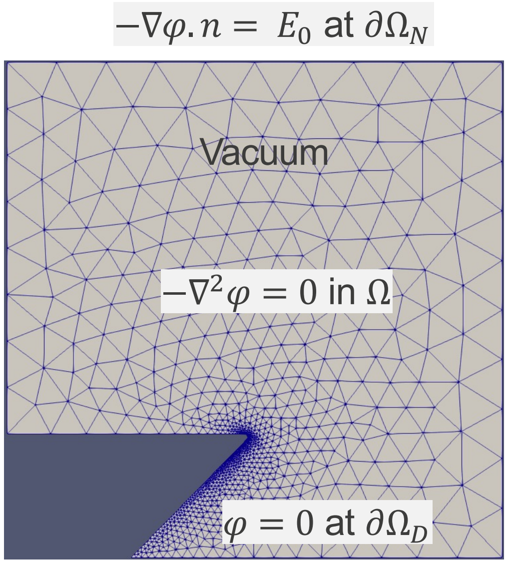
RSS enhancement due to surface steps

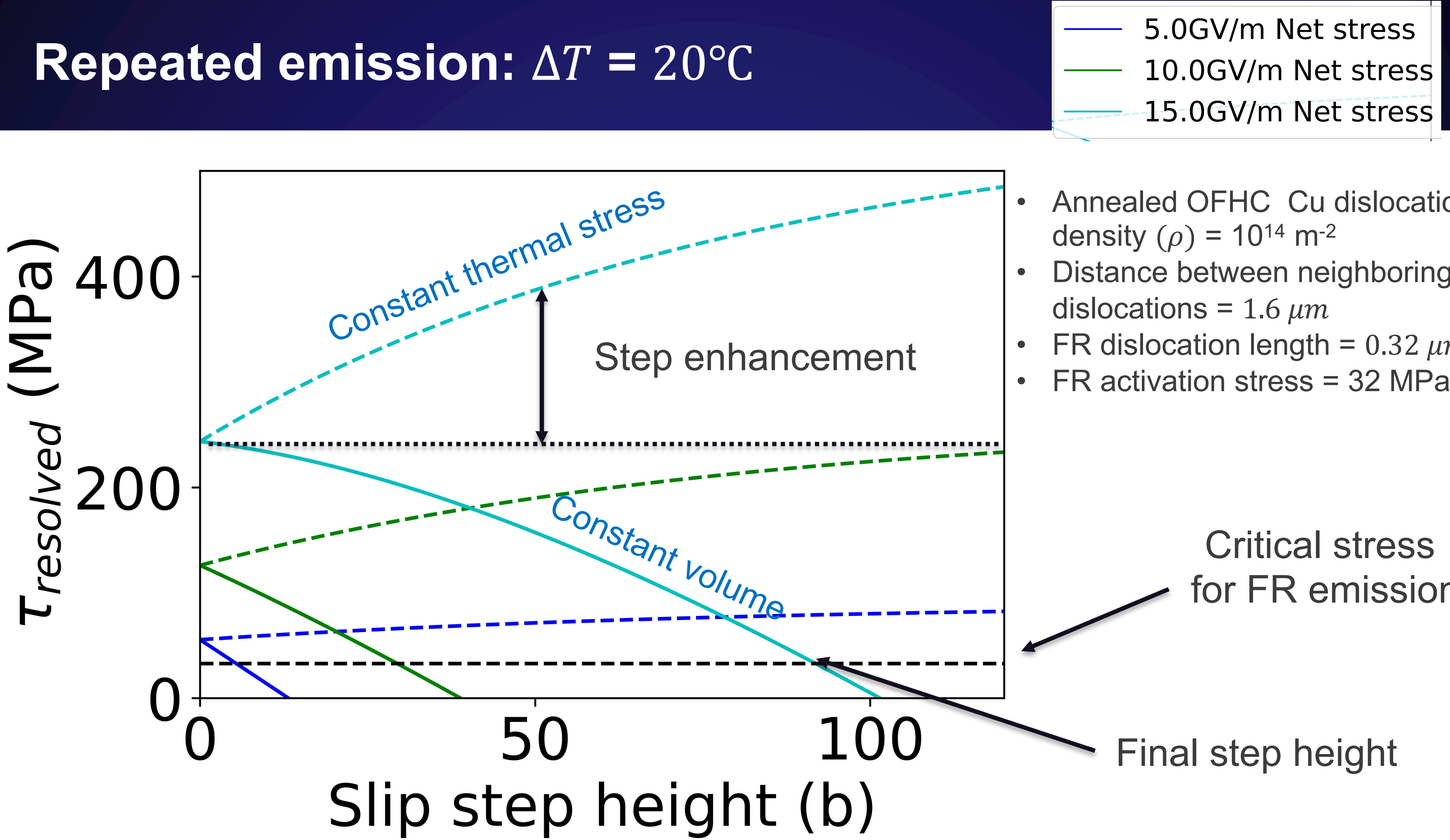




Repeated emission

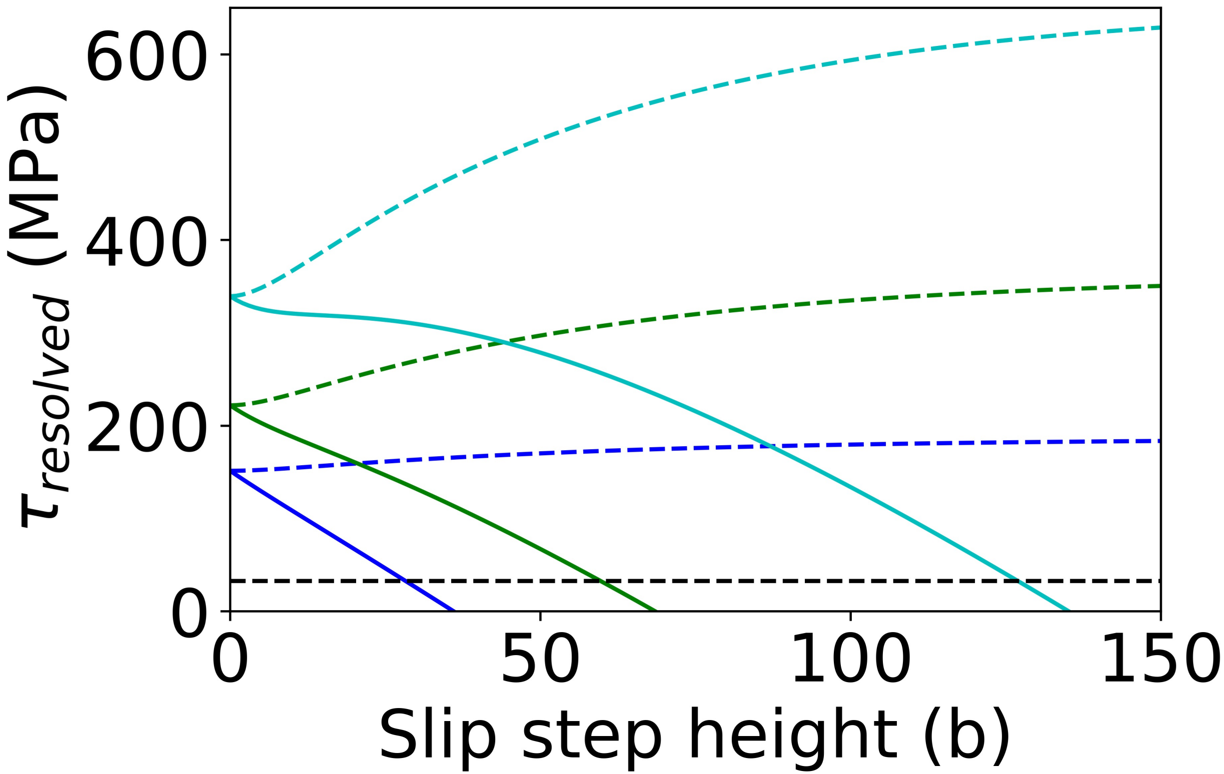
- At fixed thermal stress, the FR source could emit indefinitely
- At fixed volume, the source gradually exhausts itself, as the plastic strain relaxes the driving force from the thermal stress
- What is the impact of E on the final step height?

Repeated emission: ΔT = 20°C



- Annealed OFHC Cu dislocation density (ρ) = 10^{14} m^{-2}
- Distance between neighboring dislocations = $1.6\ \mu m$
- FR dislocation length = $0.32\ \mu m$
- FR activation stress = 32 MPa

Repeated emission: ΔT = 80℃



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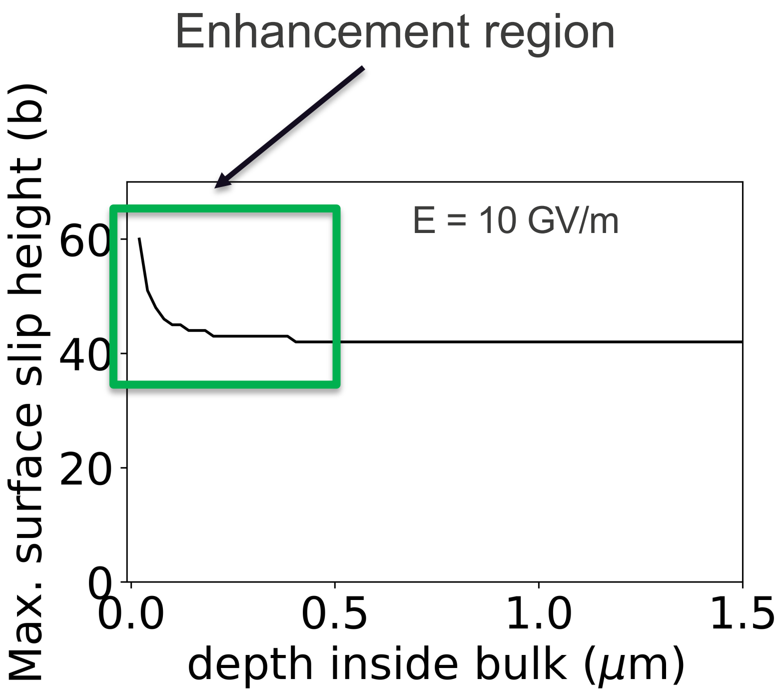
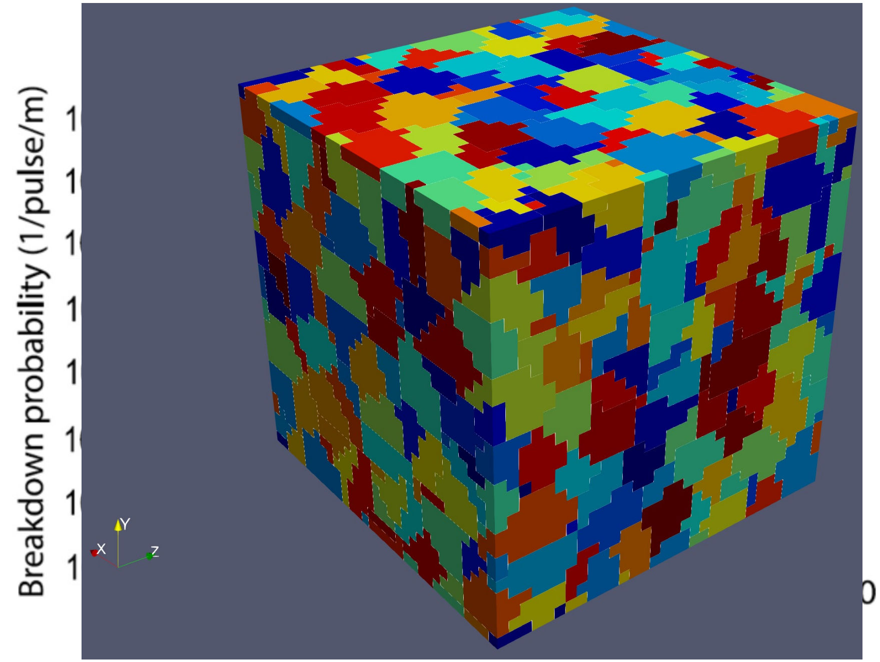
Repeated emission: step enhancement

- Electric fields can assist in dislocation emission, at very high fields. Small effect at typical gradients.
- Thermal stresses from RF losses main driving force
- Field coupling with surface steps can enhance dislocation emission at short range (~1 μm, comparable to RF heating range) and high field
- **Could play a role in near-breakdown conditions**

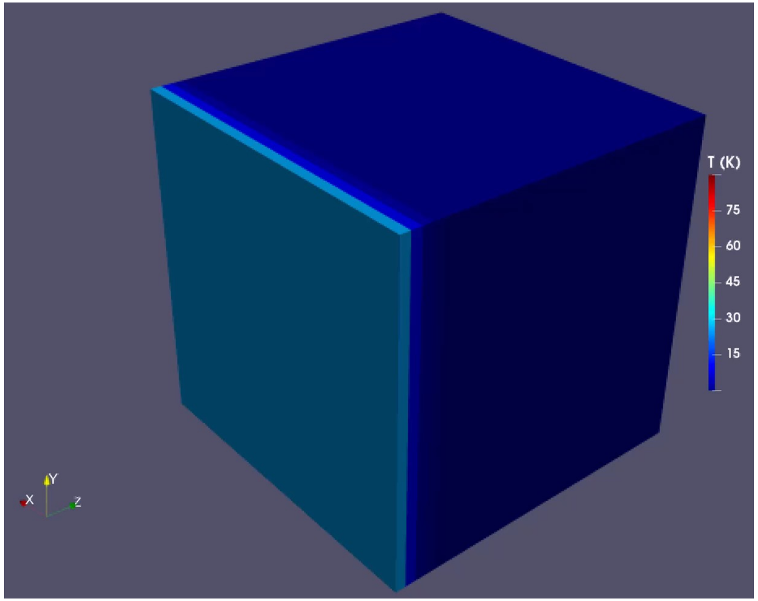


In progress: Crystal Plasticity

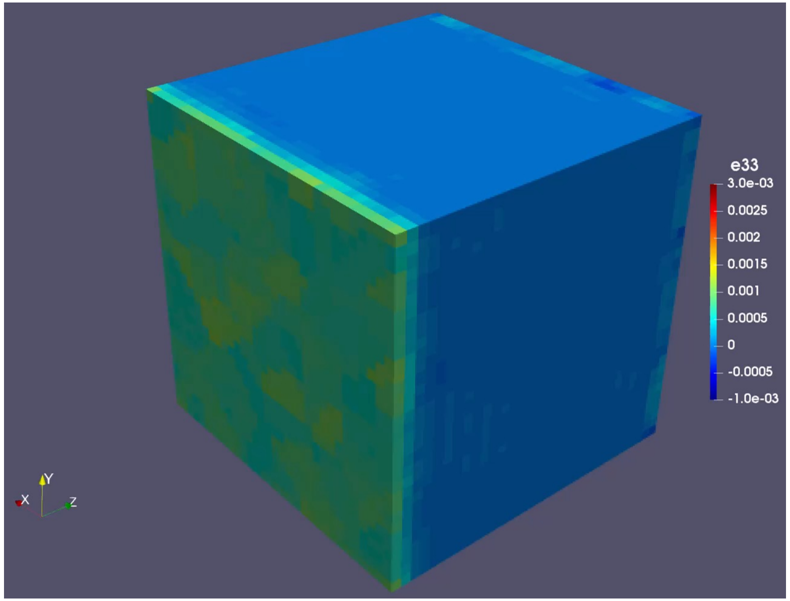
- Microstructure plays a role in breakdown
- Very difficult to capture such effects with MD, analytic models require lots of assumptions
- Currently implementing coupled thermo-plastic solver to better understand surface deformation
- Future task: include E coupling



In progress: Crystal Plasticity



Temperature distribution



Plastic strain distribution

Conclusion

- We have developed an accurate, all-atomistic, method to include E in classical MD simulations
- We have applied this technique to the coupling of E with FR plasticity through surface features.
- High local fields are required for significant enhancement. Could play a role near breakdown.

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