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

- Plastic deformation in real materials is extremely complex
- Heroic efforts to model evolution of dislocation distribution under field [e.g., MDFF by Ashkenazy et al.]
- Important takeaway: key parameter is $\beta$, 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 $N_{\text{electrons}}^3$)
  • 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
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

Coupling with structure: concentration, shielding

E = -0.4 GV/m

Induced charges

Polarization
Validation: no polarizability, no intrinsic dipole
Validation: polarizability, no intrinsic dipole
Validation: polarizability, intrinsic dipole
Intrinsic dipole

![Graph showing intrinsic dipole with V_{classical} and V_{DFT} curves.](image-url)
Validation Cu/Ag: polarizability, intrinsic dipole

![Graph showing the relationship between $V_{\text{classical}}$ (eV) and $V_{\text{DFT}}$ (eV).]
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
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 $\sim 1/r$

\[ \sigma \sim \epsilon E \sim 0.45 \text{ GPa} \]

(Cu)
RSS enhancement due to surface steps

Continuum limit from FEM

\[-\nabla \varphi \cdot n = E_0 \text{ at } \partial \Omega_N\]

\[-\nabla^2 \varphi = 0 \text{ in } \Omega\]

\[\varphi = 0 \text{ at } \partial \Omega_D\]
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?
Constant thermal stress

Constant volume

Critical stress for FR emission

Final step height

Step enhancement

Annealed OFHC Cu dislocation density ($\rho$) = $10^{14}$ m$^{-2}$

Distance between neighboring dislocations = 1.6 $\mu$m

FR dislocation length = 0.32 $\mu$m

FR activation stress = 32 MPa
Repeated emission: $\Delta T = 80^\circ C$

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