Atomistic modeling of the coupling between electric field and plastic deformation

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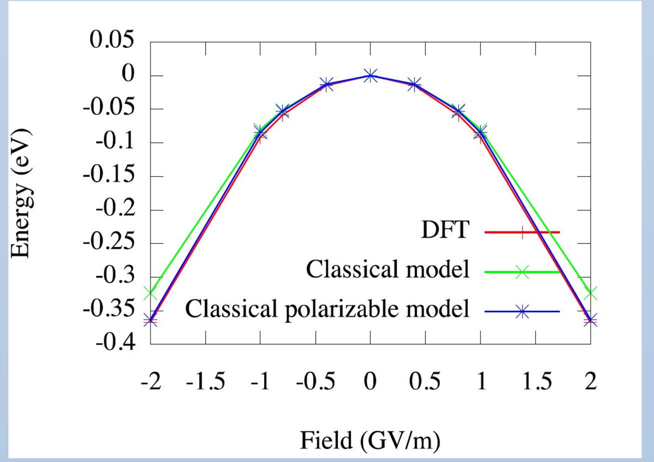
14th International workshop on Breakdown Science and High Gradient Technology (HG2022) May 16-19

Motivation

- High electric fields are inevitably encountered in several technological applications ranging from low-cost compact linear accelerators to miniaturized electronic devices.
- Material deformation in field-exposed surfaces can lead to damage growth and plasma formation ultimately resulting in **the onset of device breakdown**.
- Experiments in past have mostly been able to capture post-breakdown signatures.
- Atomically resolved simulation capabilities can provide mechanistic insight towards the early stages of breakdown formation, hence accelerating the design of **robust breakdown-tolerant metals and alloys**.
- **Material evolution under electric fields** to capture damage growth requires scale bridging e.g. from quantum mechanical DFT to classical MD simulation and then to continuum level frameworks.

Charge Equilibration based Molecular Dynamics (QEq-MD)

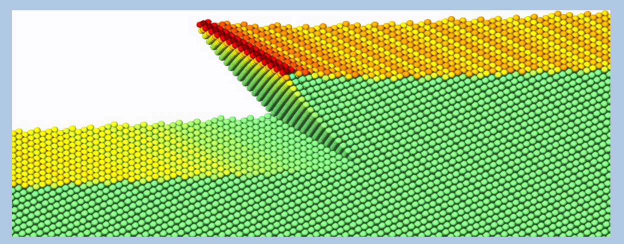
Comparison of the energy of a (100)-oriented Cu slab, obtained by DFT and by classical models.



Charges are redistributed to minimize the total electrostatic energy with a total charge conservation constraint.

Introducing virtual charge acceptors and donors, the self energy of the atoms is approximated to reproduce the quantum electrostatic energy of the system under external electric field.

Field-induced charge distribution showing a higher concentration near surface discontinuity relative to the shielded and internal regions



For an EAM Cu we express the electrostatic part of the Hamiltonian as

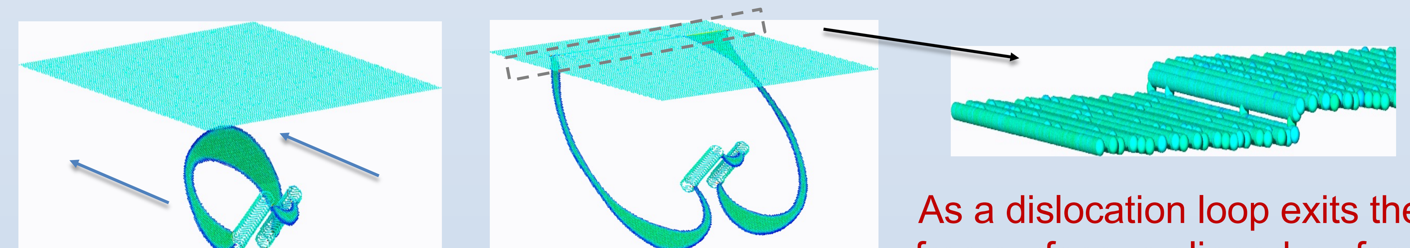
$$V_{QEq}(\boldsymbol{r},\boldsymbol{q}) = V_{coul} + V_{field} + V_{self}$$

where, $V_{self}(r,q) = \sum_i (\chi_i q_i + \frac{1}{2} J_i q_i^2)$ under the constraint $\sum_i q_i = Q_{total}$. A damped dynamics algorithm is used to solve the long-range minimization problem.

E-field Effect on Bulk Dislocation Activation

Dislocation Multiplication via Frank-Read Sources

Under a combination of electric fields and thermo-mechanical loading FR multiplication can lead to slipped surface step formation which can further enhance local electric-fields and stresses.

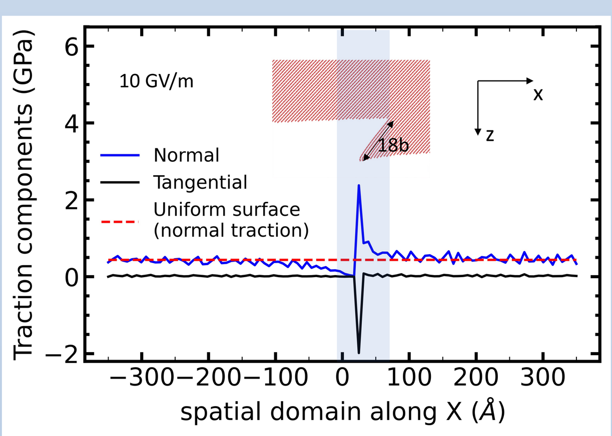


Edge dislocation pinned by cylindrical obstacles starts to bow–out under sufficient resolved shear along $[1\bar{1}0](111)$

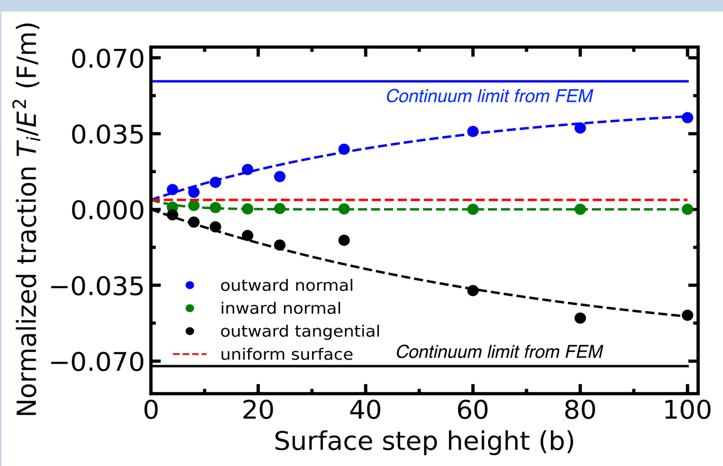
As a dislocation loop exits the free surface, a slipped surface step is formed which grows with further loop emission

Field-induced Stress enhancement

Shaded region highlights the sharp change in field-induced traction magnitude due to the presence of slip step



Peak traction magnitudes grow and eventually saturate with the increase in step-height

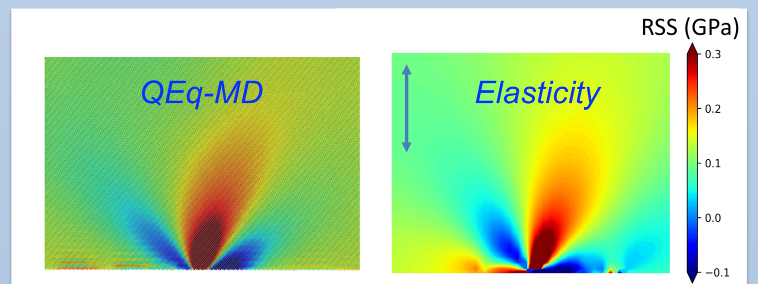


QEq-MD and Elasticity

Plane-strain half-space elasticity solution under tractions T_i

$$\sigma_{zz} = -\frac{2}{\pi}\int \frac{z^2(zT_z(s) + (x-s)T_x(s))}{(z^2+(x-s)^2)^2} ds$$

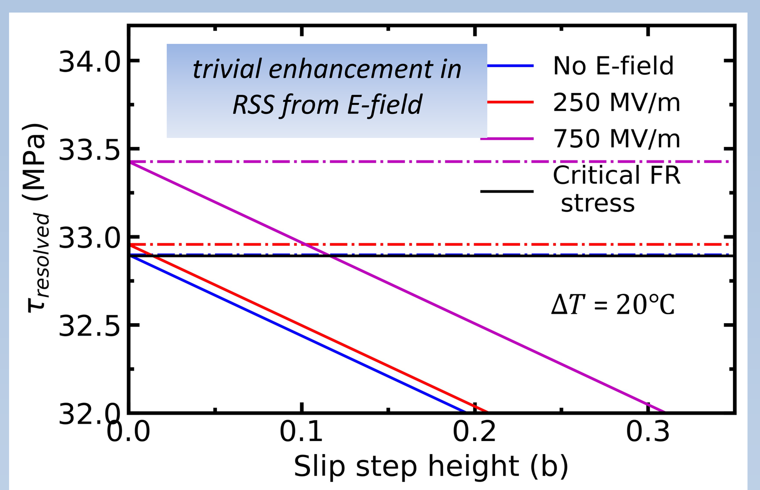
$$\sigma_{xx} = -\frac{2}{\pi}\int \frac{(z-s)^2(zT_z(s) + (x-s)T_x(s))}{(z^2+(x-s)^2)^2} ds$$



Resolved shear stress (RSS) in inside bulk with *surface step of 18b high* under *10GV/m E-field*

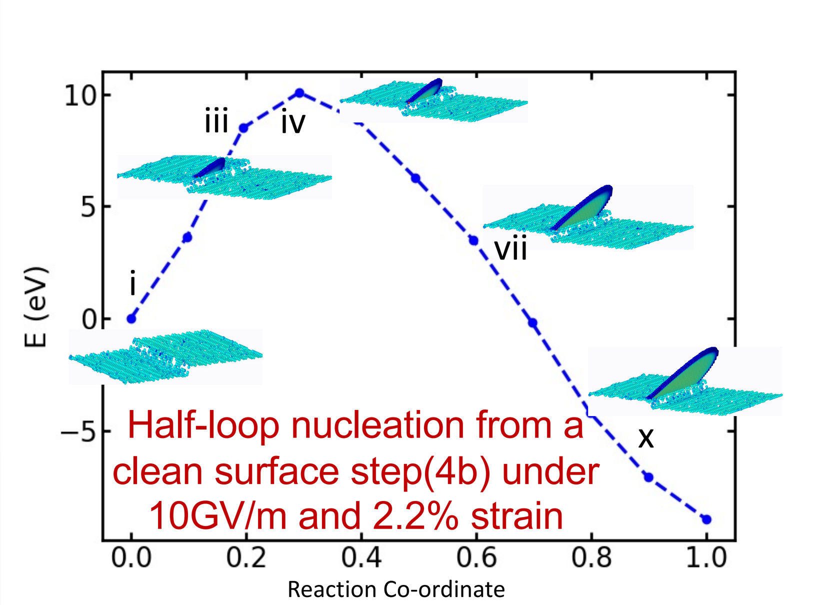
Thermal stresses can also promote surface damage

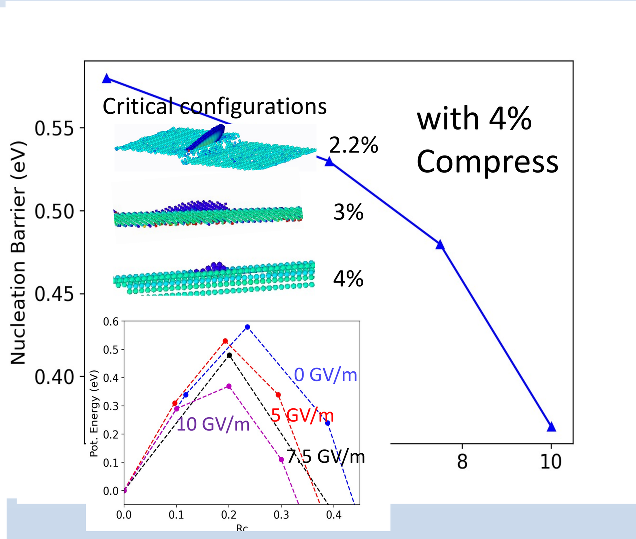
Under initially low E-fields, thermal stresses due to RF heating at even low temperature rise e.g., 20K-40K can play a key role to activate emissions at typical fields.



Surface Nucleation of Dislocations under E-fields

High stress concentration near surface steps can also lead to nucleation of dislocation half-loops from surface in absence of any bulk sources. Fixed-end nudged elastic band (NEB) simulations are performed to quantify activation barriers under electric field and thermo-mechanical stresses typically observed in field driven devices.





Nucleation barrier and critical loop radius (saddle point structures) decreases significantly with increasing E-field and strain)

Conclusions

- Charge-Equilibration based molecular dynamics simulations can capture the localized stress enhancement near slipped surfaces due to electric fields.
- While stronger E-fields magnify localized step growth in short range, it is the thermal stresses due to RF losses which govern loop emissions from bulk at typical E-fields
- Surface nucleation of dislocation half loops under external E-fields is shown to be favorable with higher external strain which may arise due to resistive heating and related thermo-mechanical sources.

References

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Acknowledgement

We gratefully acknowledge funding from LANL-LDRD-DR-2020057 and LANL-IC for the supercomputing resources.