# Nanomechanics Simulation Toolkit: Dislocations Make or Break Materials

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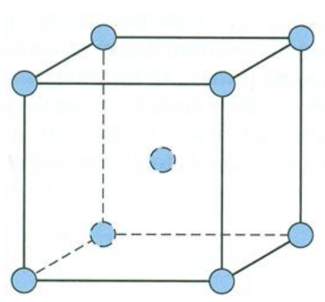
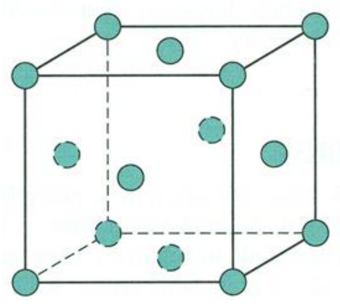
## Background

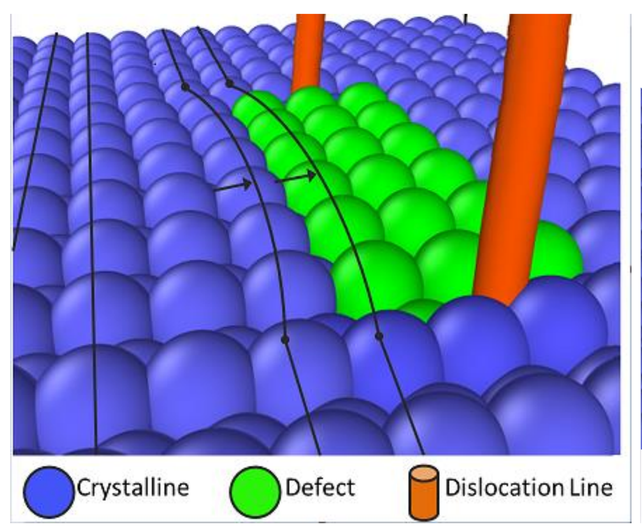
- Dislocations, or atomic linear defects in crystal structures, dictate much of the mechanical response of materials
- No current predictive dislocation analysis tool on the nanoHUB
- Simulation tools such as Molecular dynamics solve for the movement of atoms, and in turn the dislocations



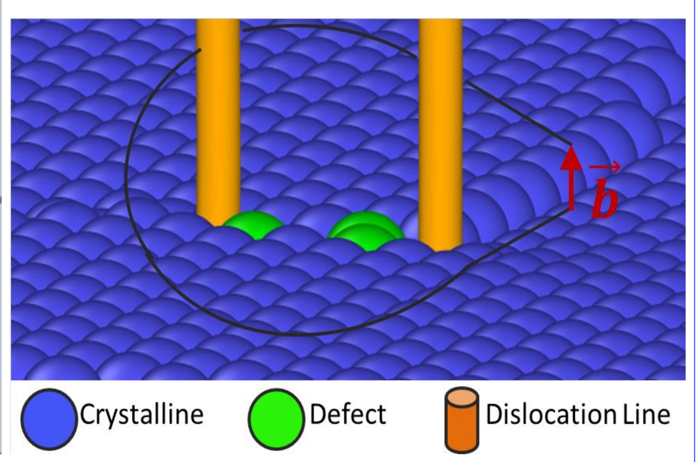
**(Left)** BCC crystal (Fe)[1]

**(Right)** FCC crystal (Cu)





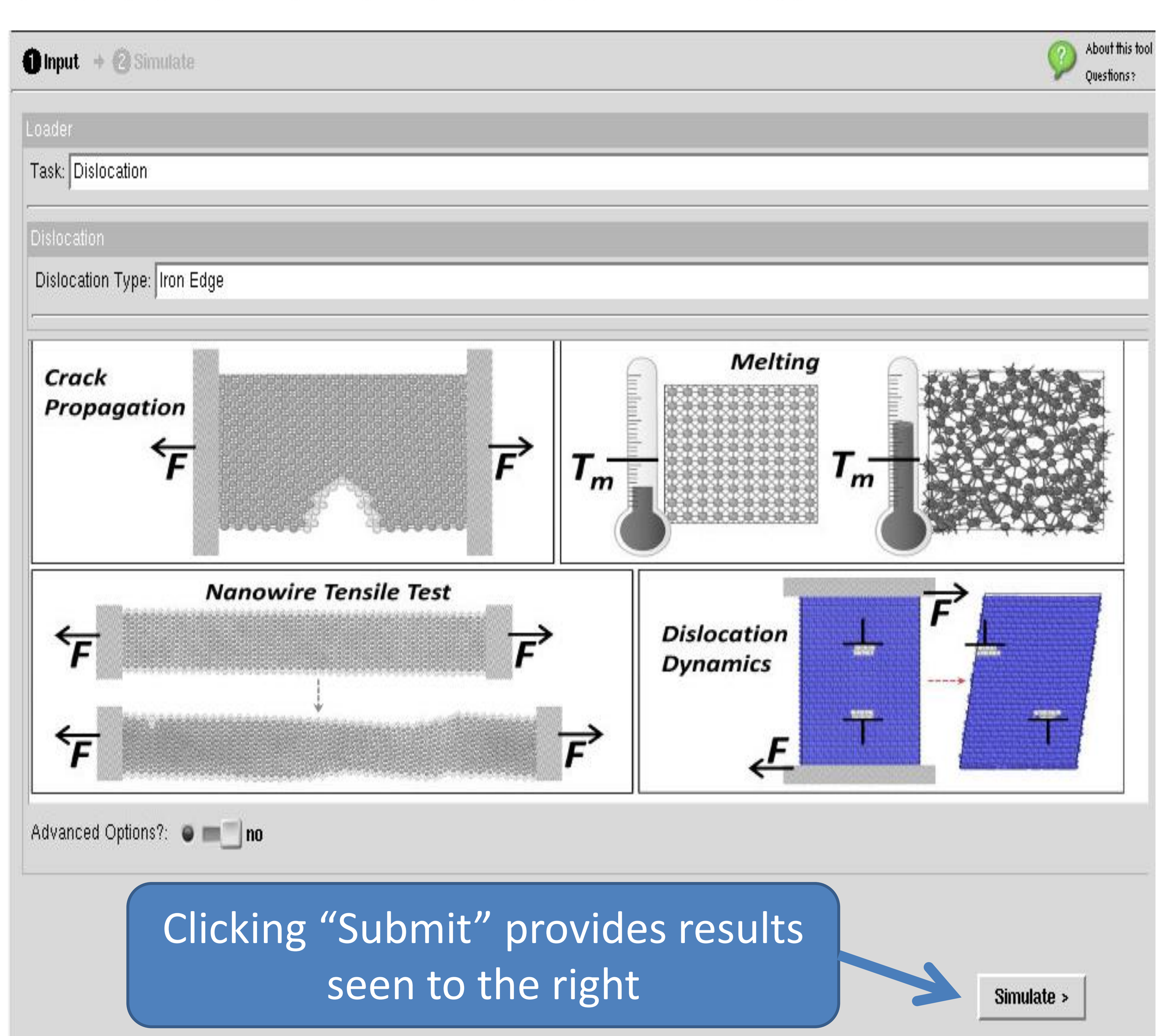

**Edge Dislocation[2]**




**Screw Dislocation[2]**

## Graphical User Interface(GUI)

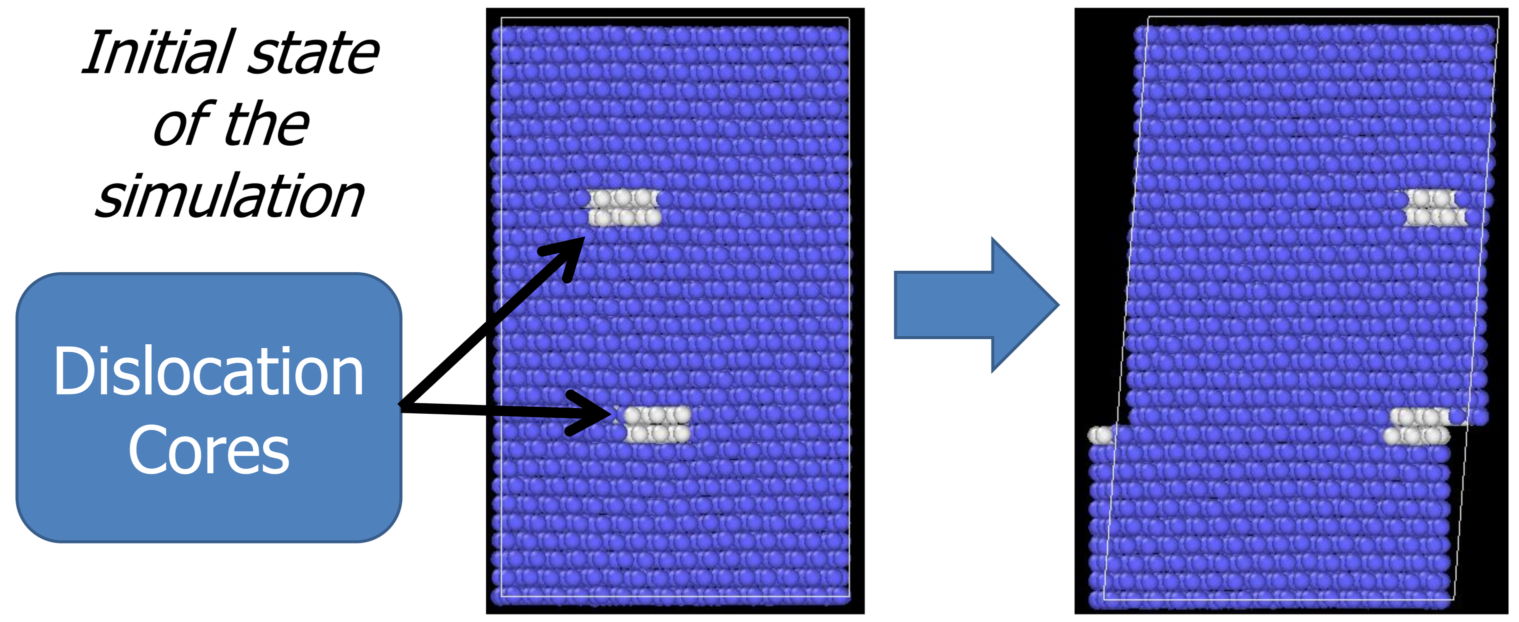
- Our objective aims to create a GUI to enable wide spread use of simulation tools to predict the behavior of defects in metals




## Simulation results of edge dislocation movement

**https://nanohub.org/tools/nanomatmech**

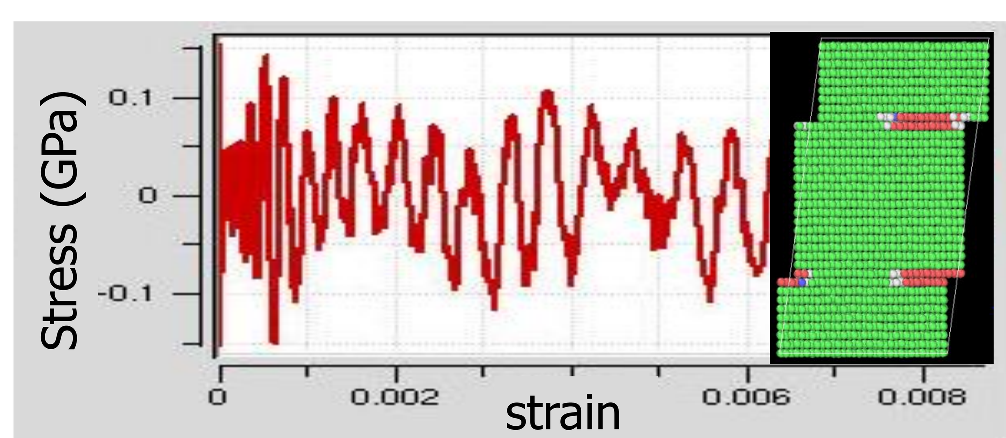
*Initial state of the simulation*



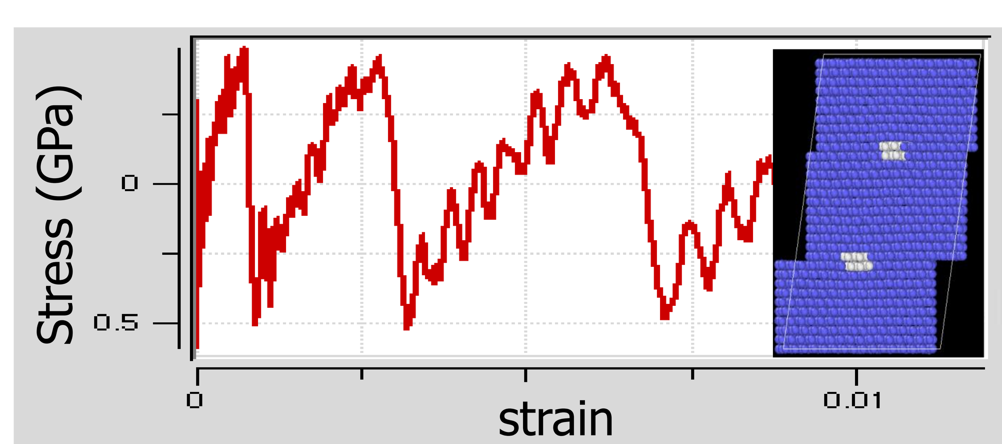

*Final state of the simulation where the applied shear moves the dislocation. Defects are created and simulated using the LAMMPS[4] simulation package.*

## Characterizing Defects using MD

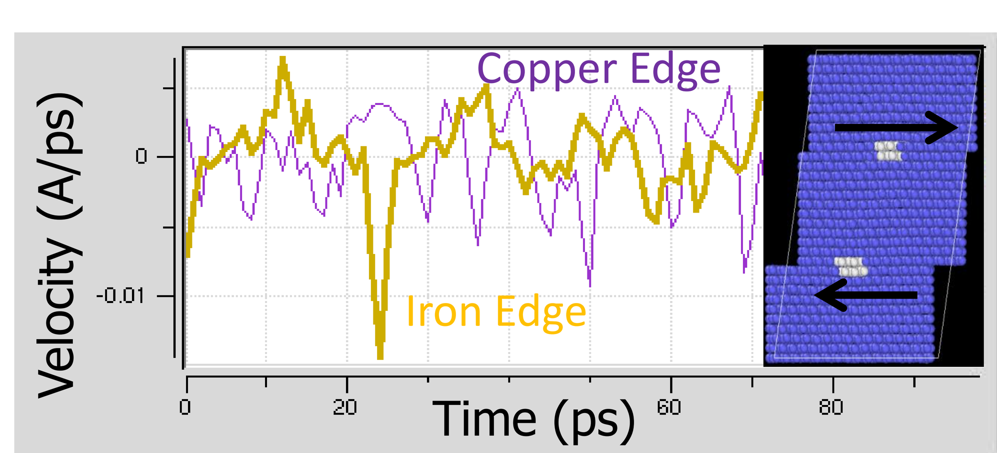
*Dislocation Motion (Resolved Shear Stress)* vs. *Dislocation Nucleation (No Resolved Shear Stress)*



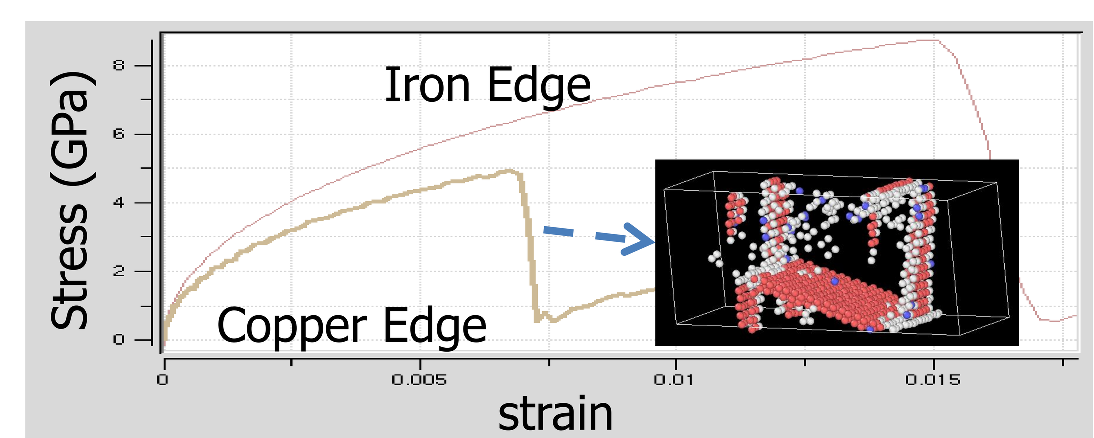

**Edge Dislocation FCC Copper[3]** – Oscillation around 0 GPa conveys gliding motion



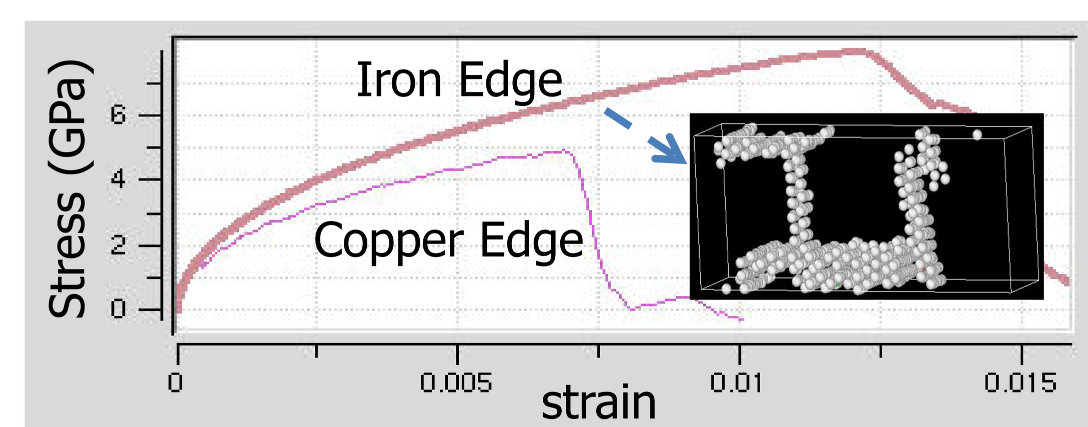

**Edge Dislocation BCC Iron[3]** – Increasing stress implies single dislocation takes more stress to move than two partials in a FCC crystal



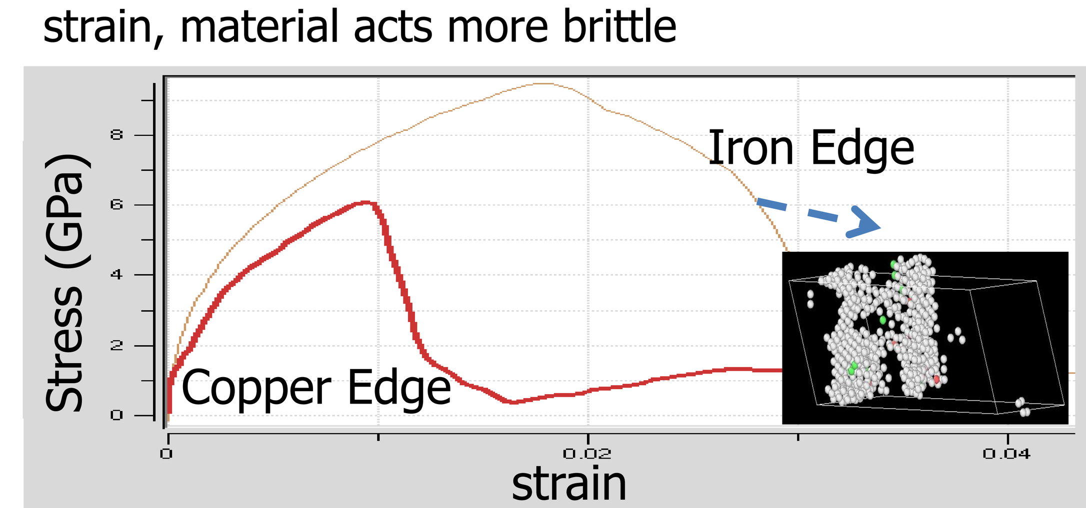

**Edge Velocities[3]** – Dislocation cores move at roughly constant value for constant shear rate




**Fixed Strain Rate and Temperature[3]** – Different magnitudes because dislocations in Copper are partials compared to Iron. Inset shows an example nucleation event at high strain



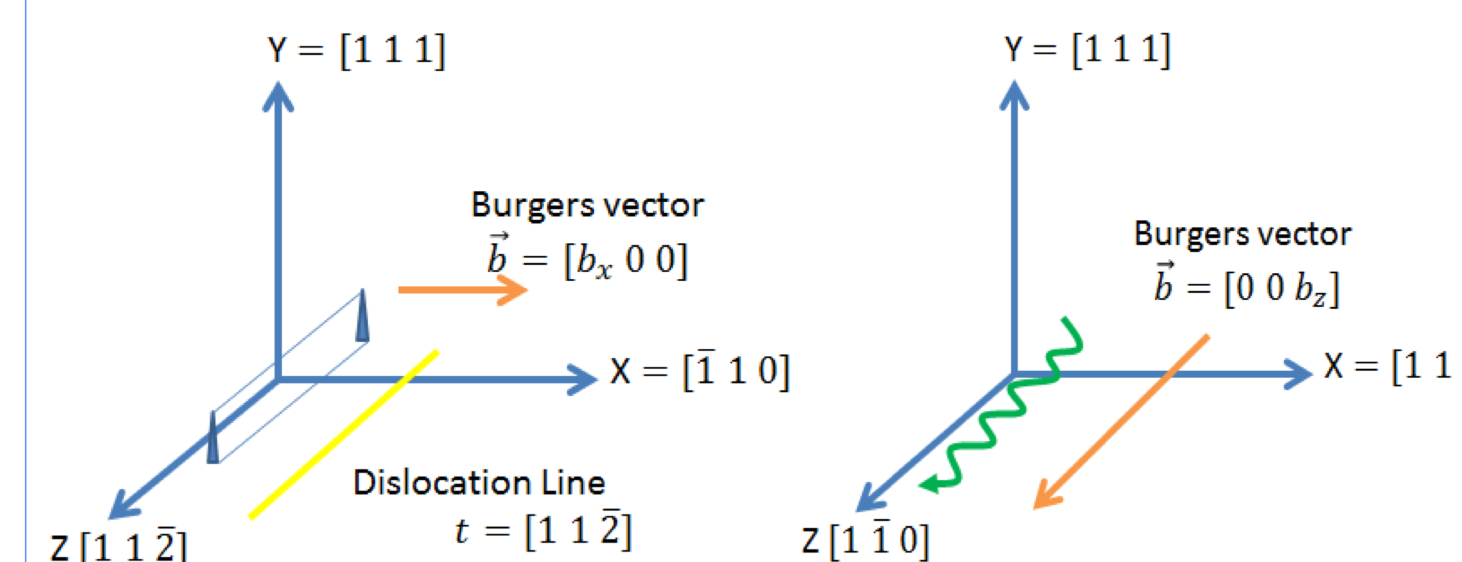

**Double Strain Rate[3]** – Yielding occurs at lower strain, material acts more brittle




**Reduced Temperature[3]** – Yielding occurs at much later strain, BCC material acts more brittle

## Discussion

- Dislocation type depends on relative orientation of: Burgers vector (direction of atom shift), dislocation line and slip plane (closed packed)
- Dot product of the applied shear stress aligns with the slip plane is known as resolved stress (i.e. what moves the dislocation)




**FCC Edge Dislocation** **FCC Screw Dislocation**

## Conclusion

- Dislocation behavior dependent on crystal and orientation
- Shear stress causes dislocations to glide or nucleate
- Replicates the behavior of bulk material by modeling at the nanoscale
- GUI presents the topic in a user-friendly manner
- Advanced users can freely create and define their own simulation parameters

## Future Work

- More materials/crystal structures
- Greater input flexibility
- Uncertainty Quantification (UQ)
- Upload user data and input files

## References

[1] Callister, William D. *Material Science and Engineering An Introduction.* York: Quebecor Versailles, 2007. Print.
[2] Ovito A. Stukowski, Modelling Simul. Mater. Sci. Eng. 18, 015012 (2010)
[3] Rappture.org
[4] LAMMPS software package (lammps.sandia.gov)

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