

Topical Overview:

Dislocations and their motion govern the plastic deformation of metallic systems. One is able to predict dislocation behavior using DD simulations; however, these simulations are not always in agreement with behaviors captured from Molecular Dynamics (MD). Using a GNN, one can determine correlation functions that will improve DD mobility laws and plastic flow rules.

Research Methodology:

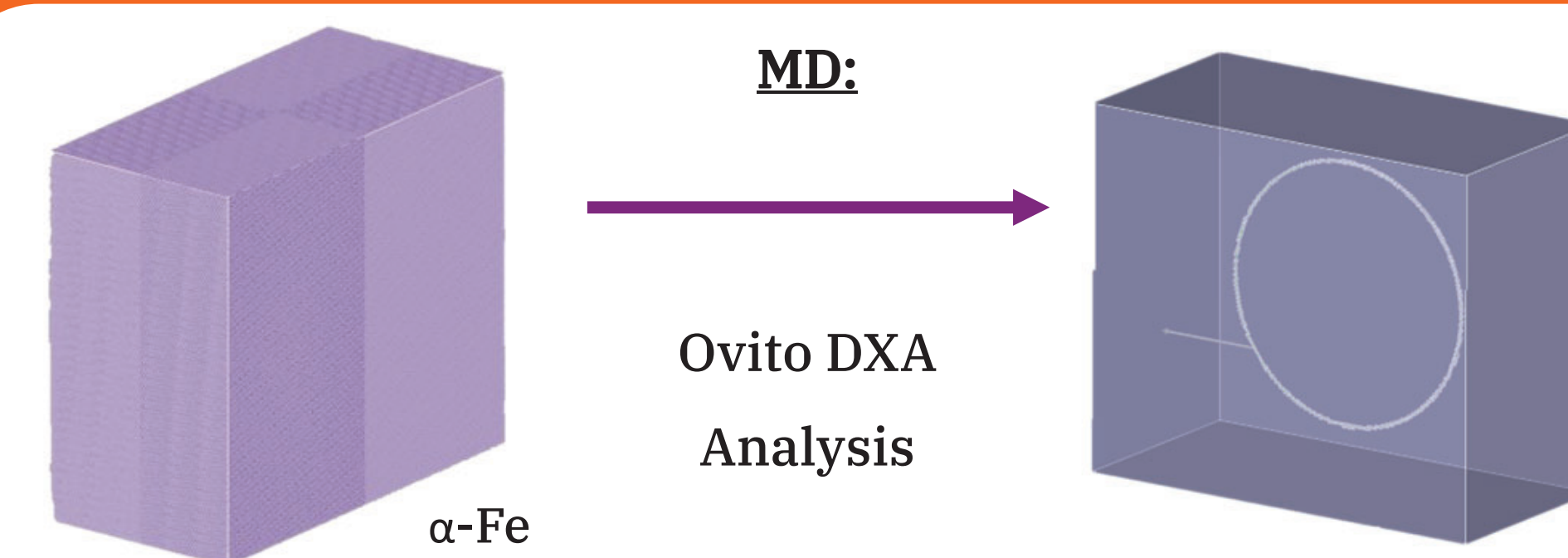
Physics Informed ML Model
(Trained to Improve DD Dynamics)

MD position evolution
passed to ML

DD stress analysis is
passed to the ML

MD Simulation
(Captures Thermal Effects)

DD Simulation
(Stochastic Estimation)



DD:
MD configurations are replicated
in DD framework and resultant
forces and stresses are computed
at discrete quadrature points
about the dislocation line

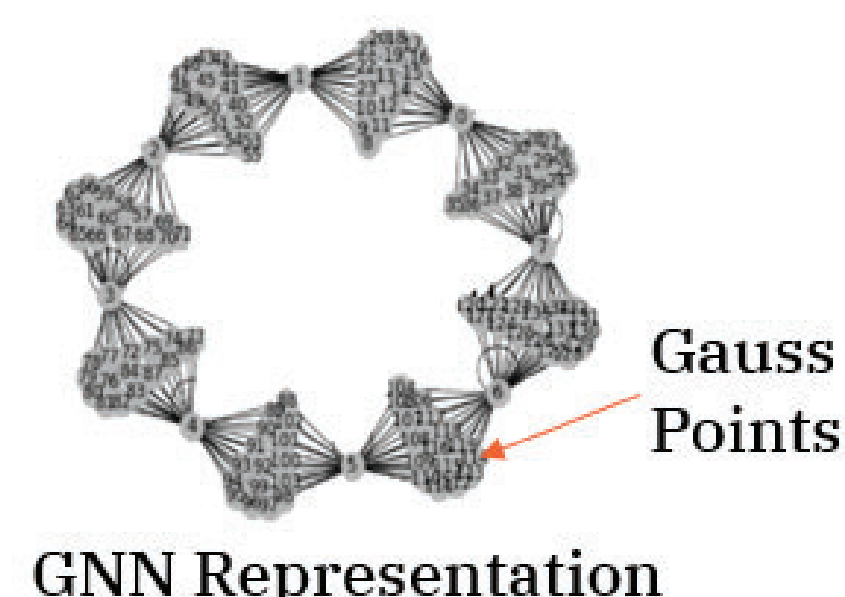
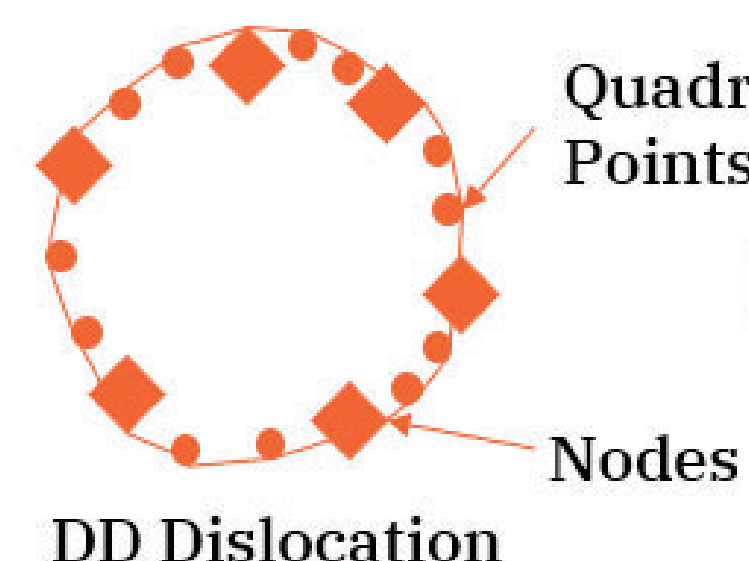


Microscale

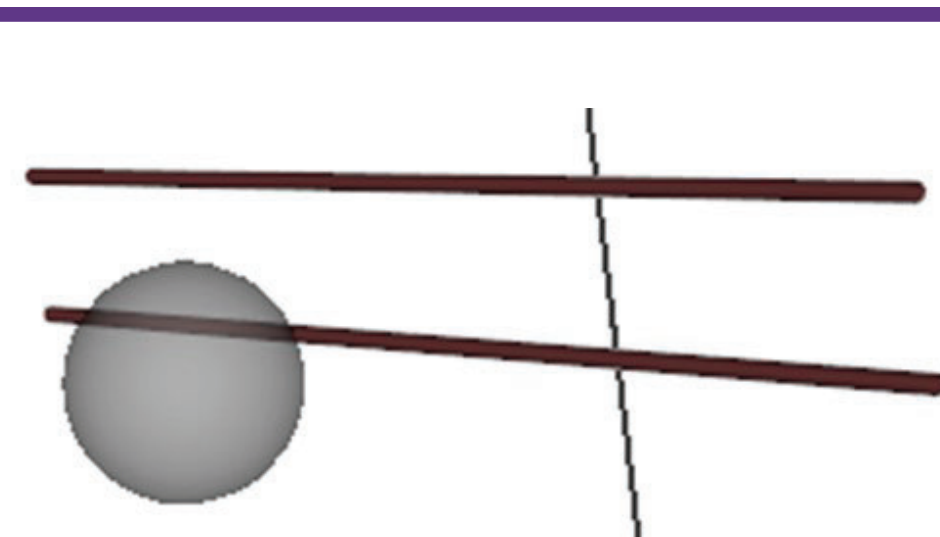
Not only does the framework tie together different dimensional scales, but all of the currently underdeveloped components of DD flow rules will be improved by MD

Mesoscale

Information Pipeline



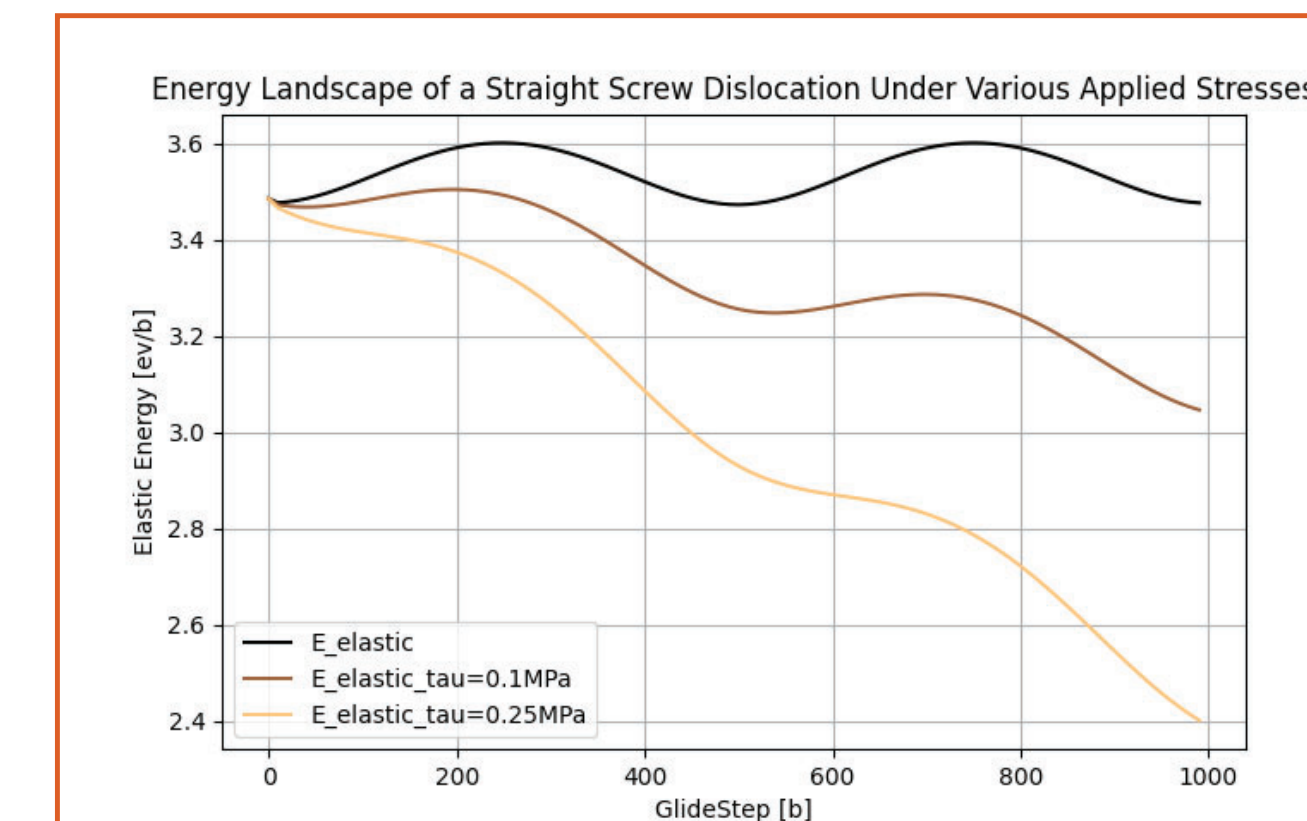
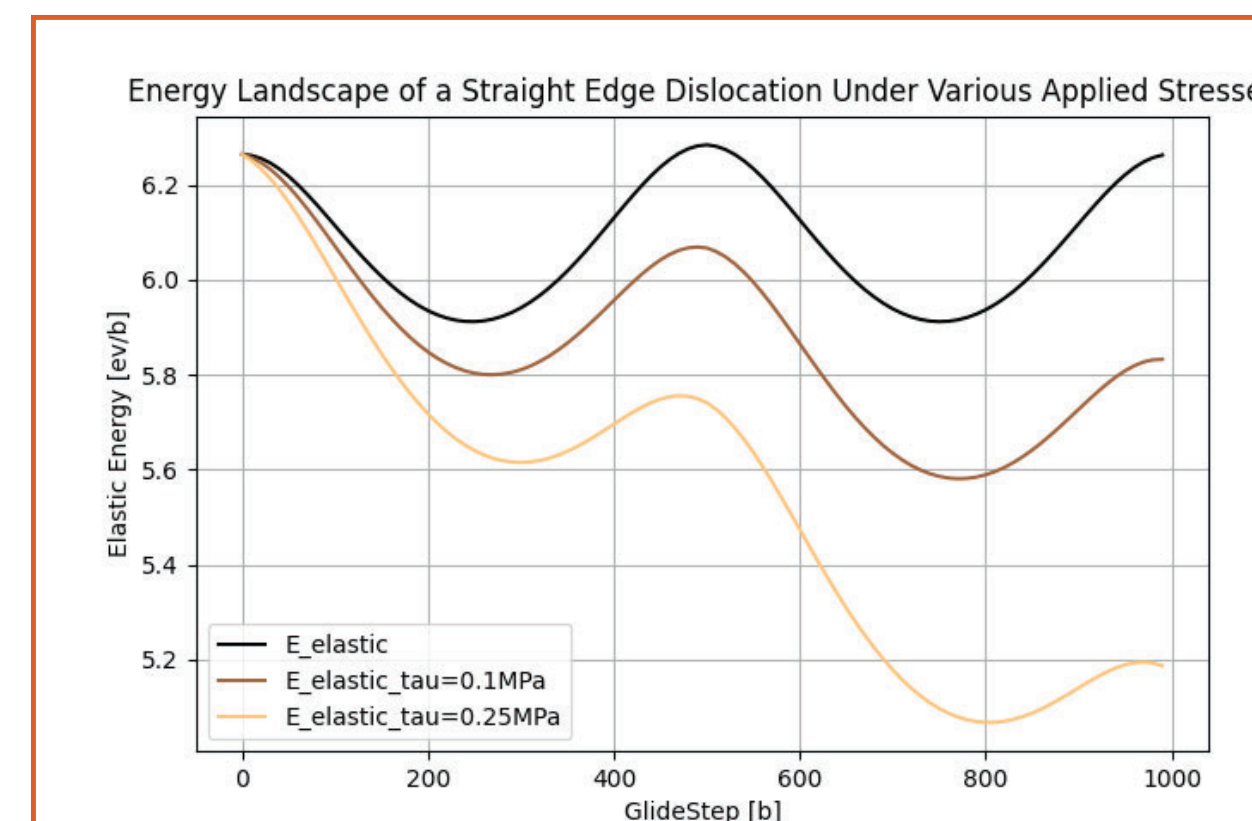
Thermally
Activated
Processes



Dislocation Interaction Study of Local Obstacles (left) Inclusions (right) Stacking Fault Tetrahedra

Results and Further Work:

Plots containing elastic energy landscapes of dislocation dipoles from MoDeLib DD simulations are provided below. Studies such as these allow us to calculate the energy barrier for certain dislocation interaction mechanisms, such as thermally activated annihilation of local obstacles.



Energy Landscape for Dislocation Dipoles of (left) Edge and (right) Screw Character
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