SAND2019-13245C

Large-Scale Molecular Dynamics (MD) Derivation of Length-Insensitive Dislocation Mobility Laws in Fe-Ni-Cr Stainless Steels

International Conference on Plasticity, Damage & Fracture

Jan. 3-9, 2020, Rivera Maya, Mexico

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Motivation

- Dislocation mobility laws are required for dislocation dynamics simulations but cannot be measured experimentally.
- Dislocation mobility in alloys is indicative of solute strengthening.
- Stainless steels are important structural materials.
- Past MD results of dislocation mobility in alloys are size sensitive.
- Mobility laws in a wide range of stresses and temperatures have not been well understood.
- **We attempt to understand size-insensitive mobility laws in a wide stress-temperature space for stainless steels.**

Goals

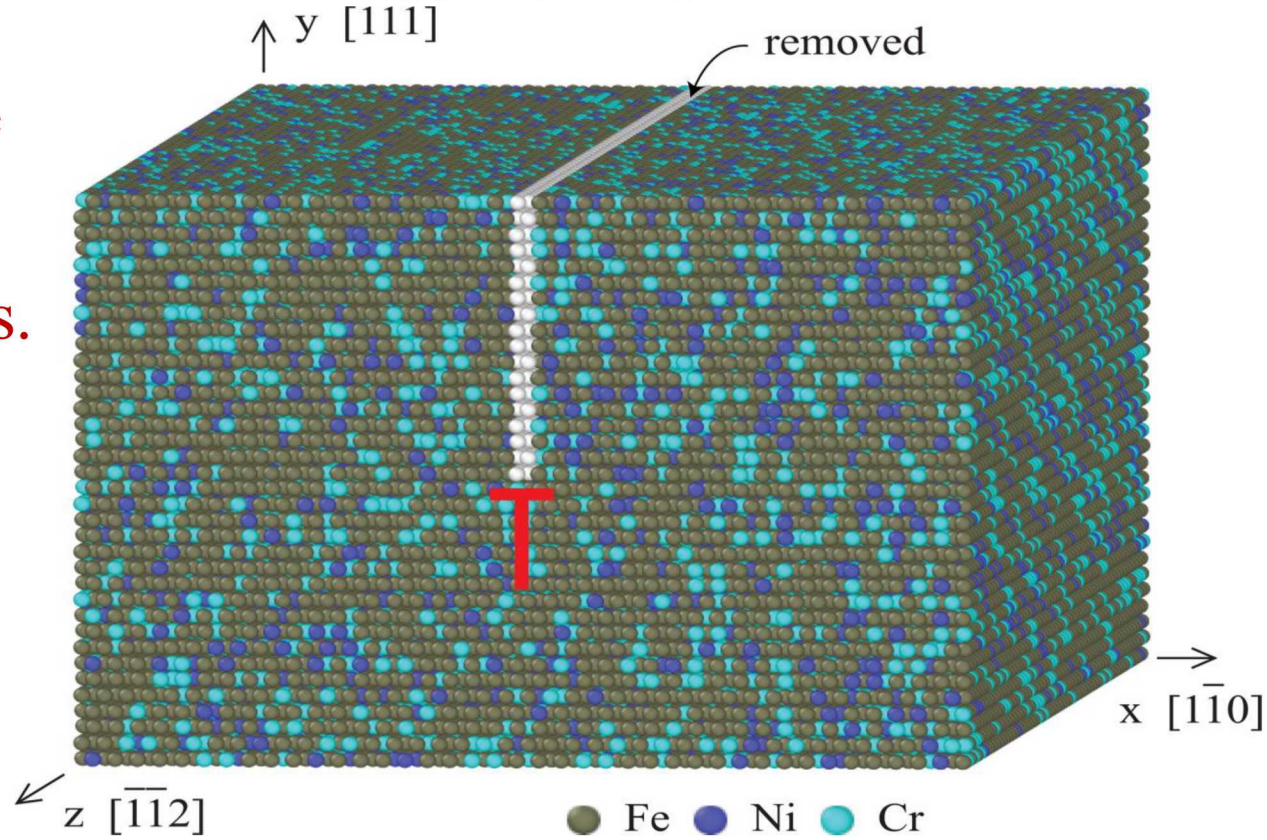
- Use MD to systematically study edge dislocation mobility in random $Fe_{0.7}Ni_{0.11}Cr_{0.19}$ over a range of stresses and temperatures.
- Develop a theoretical mobility model to rationalize the MD data.
- Understand when and why the mobility becomes length-dependent.

Approach

- Use an Fe-Ni-Cr EAM potential (Zhou et al, 2018).
- Stresses are modeled as forces on surface layers of atoms (in ±x).
- NPT simulations are performed for ≥ 8 ns.
- Dislocation distance is determined by scaling the relative shift between upper / lower halves of the crystal.
- For each stress / temperature condition, various sizes are explored.

Computational Geometry

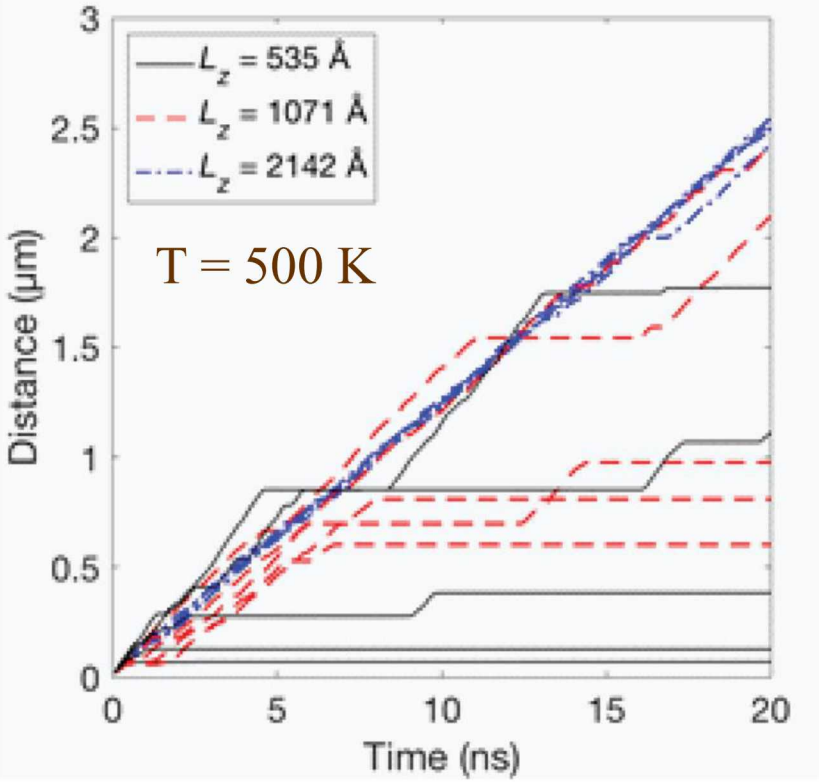
$Fe_{0.70}Ni_{0.11}Cr_{0.19}$ (~304L)



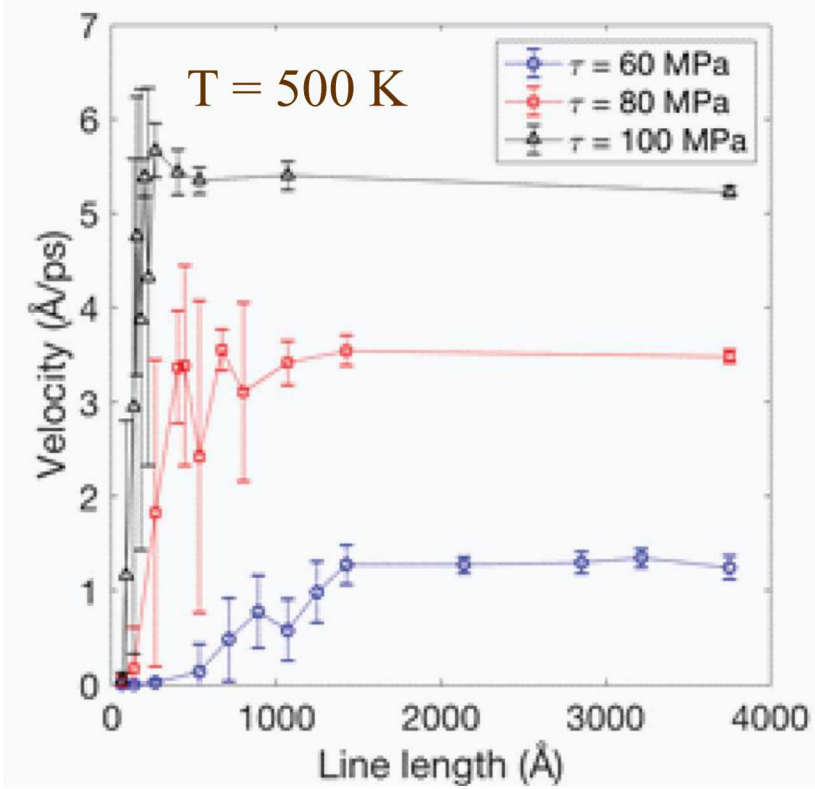
L_z: dislocation length, L_y: dislocation-surface spacing, L_x: periodic moving distance.

Size Effects

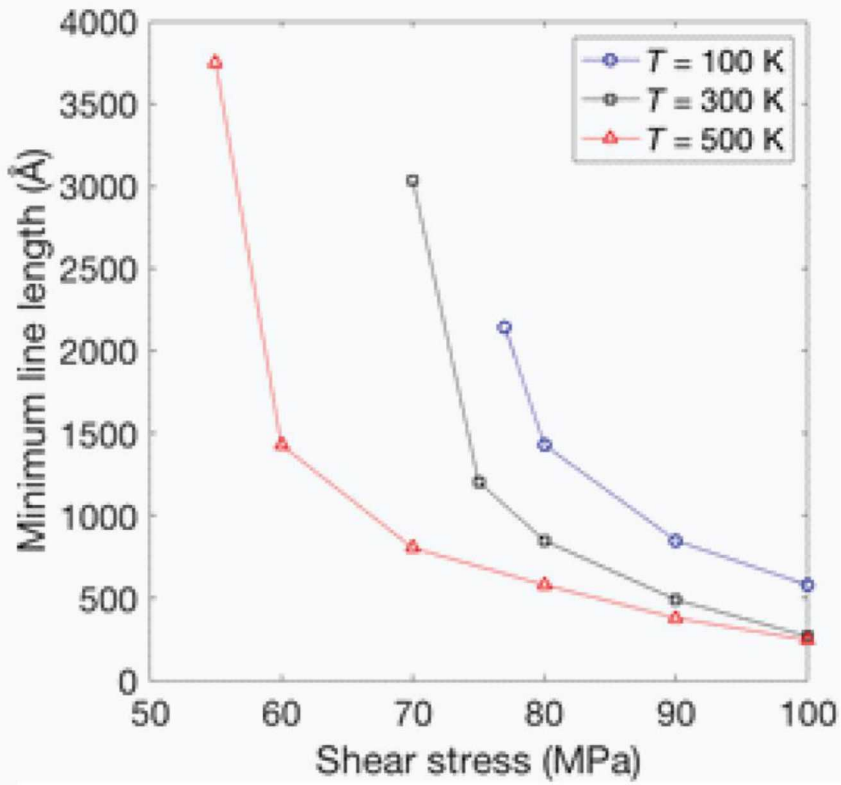
(a) distance at τ = 60 MPa



(b) velocity



(c) threshold size-independent length

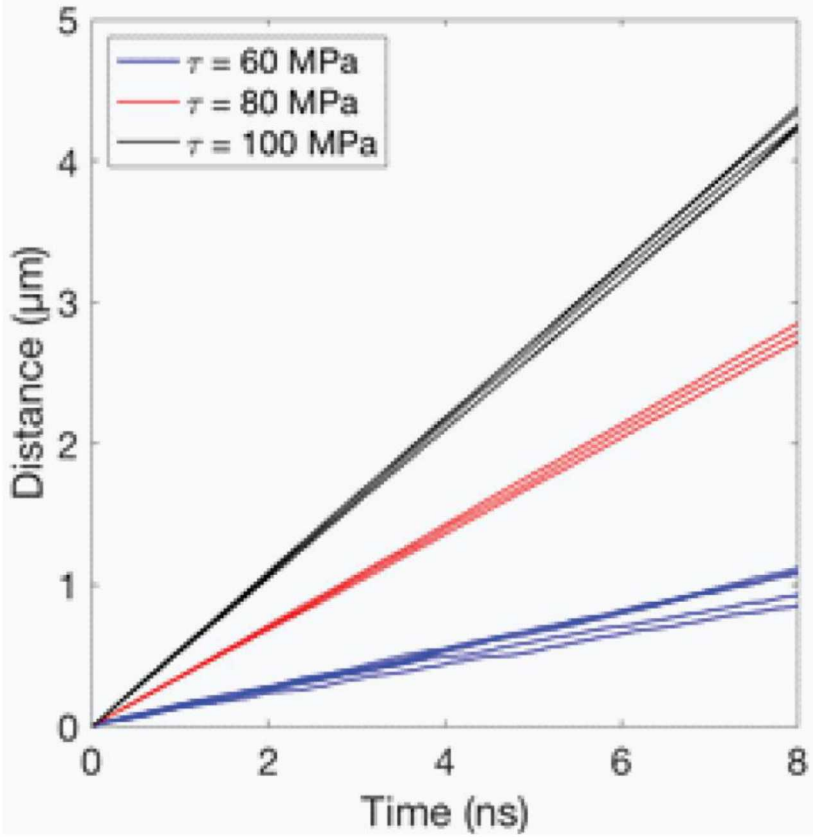


- Velocities are sensitive to dislocation length L_z but not to L_y and L_x.
- Size-insensitive velocities can be obtained at high stresses and temperatures.

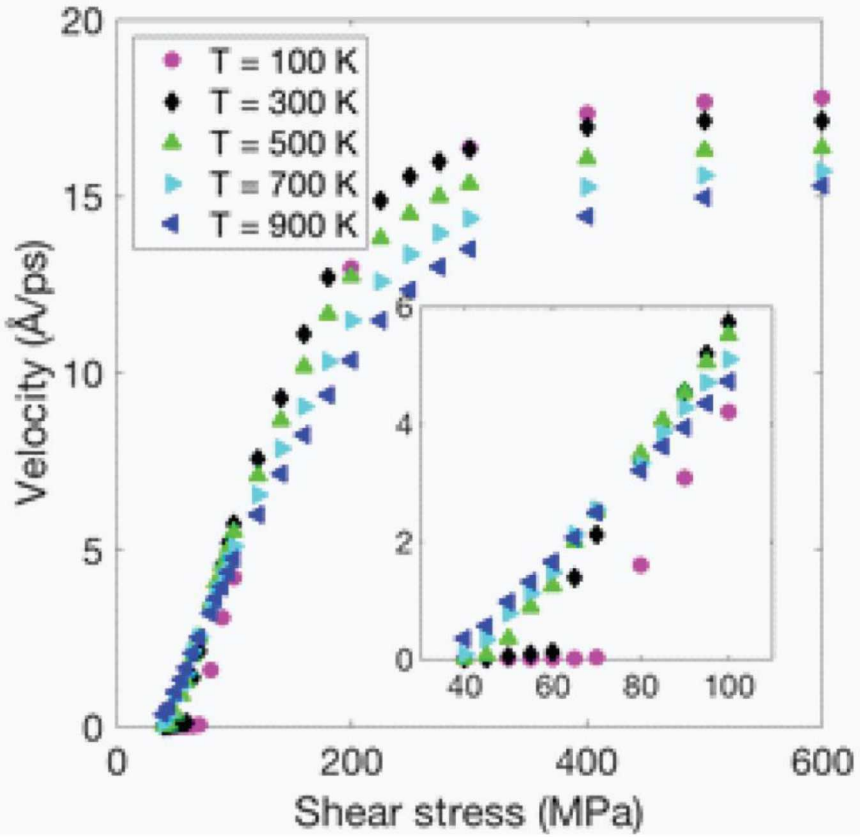
Selected Dislocation Distance/Velocity

Dislocation length L_z = 3748 Å

(a) distance at T = 500 K



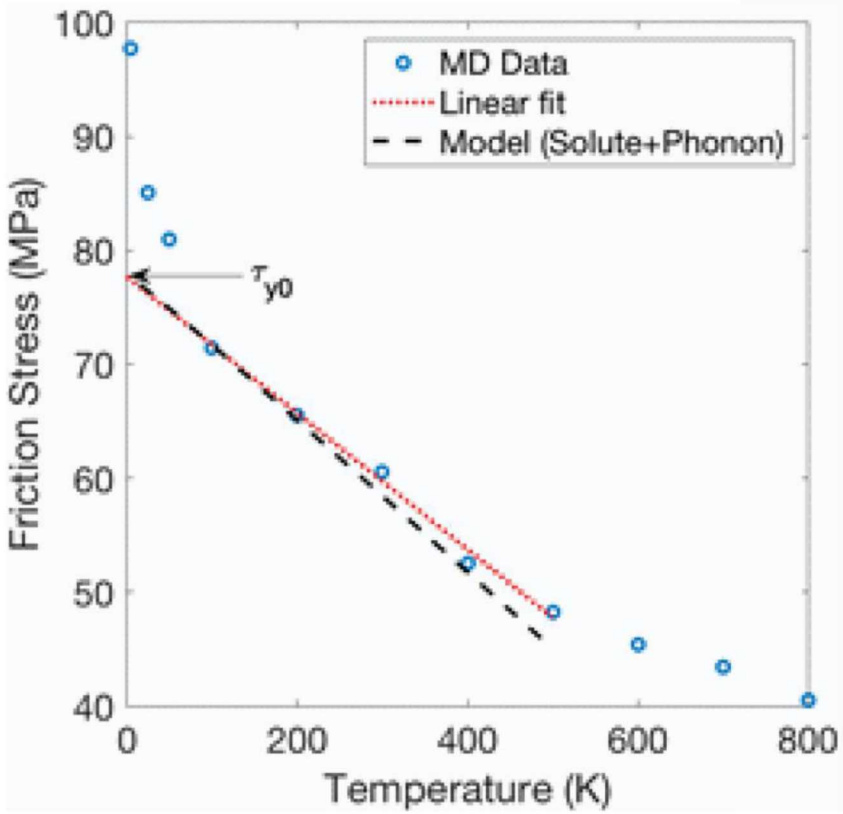
(b) velocity



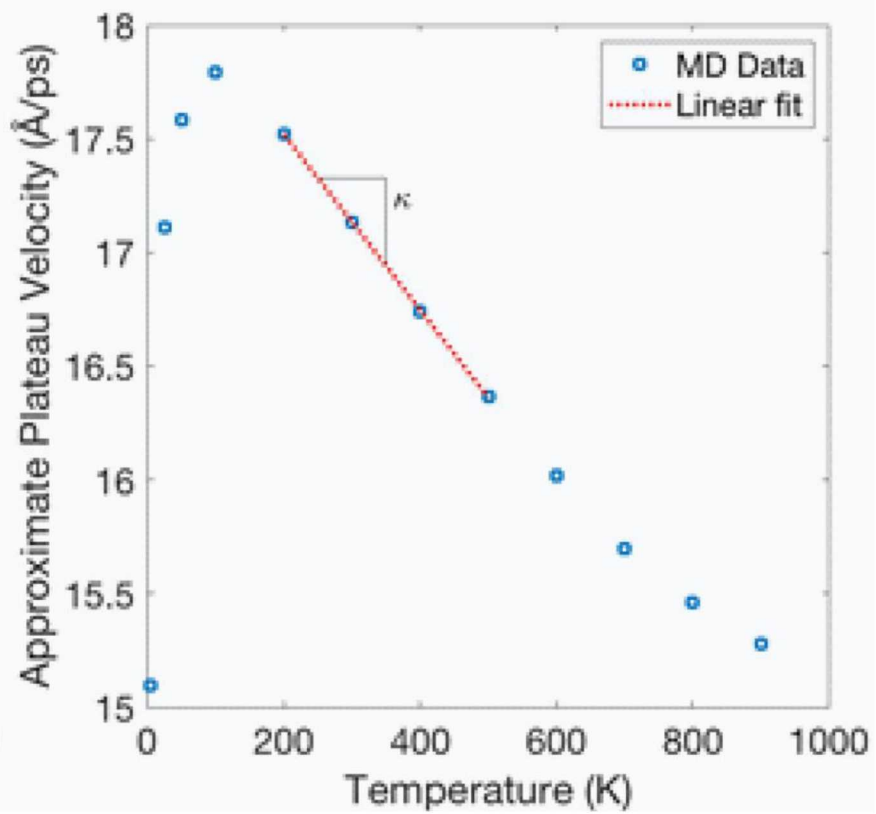
- Velocities reach plateaus at high stresses.
- At low stresses, velocities increase with temperature (solute dragging).
- At high stresses, velocities decrease with temperature (phonon dragging).
- Fraction stress (τ_f) decreases with temperature.

Friction Stress and Plateau Velocity

(a) friction stress



(b) plateau velocity at τ = 600 MPa



- Friction stress criterion: velocity $\leq$ 0.25 Å/ps.
- At intermediate temperatures, friction stress and plateau velocity both linearly decrease with temperature.

Analytical Mobility Law

Solute + Phonon only

Account for solute, phonon, and "singular" drag mechanisms:

$$\tau_d = \frac{1}{b}\left(F_{sol} + F_{ph} + F_{sing}\right)$$

$$F_{ph} = CT^n v$$

$$F_{sing} = s(c_T - v)^\beta$$

Marian and Caro, 2004.

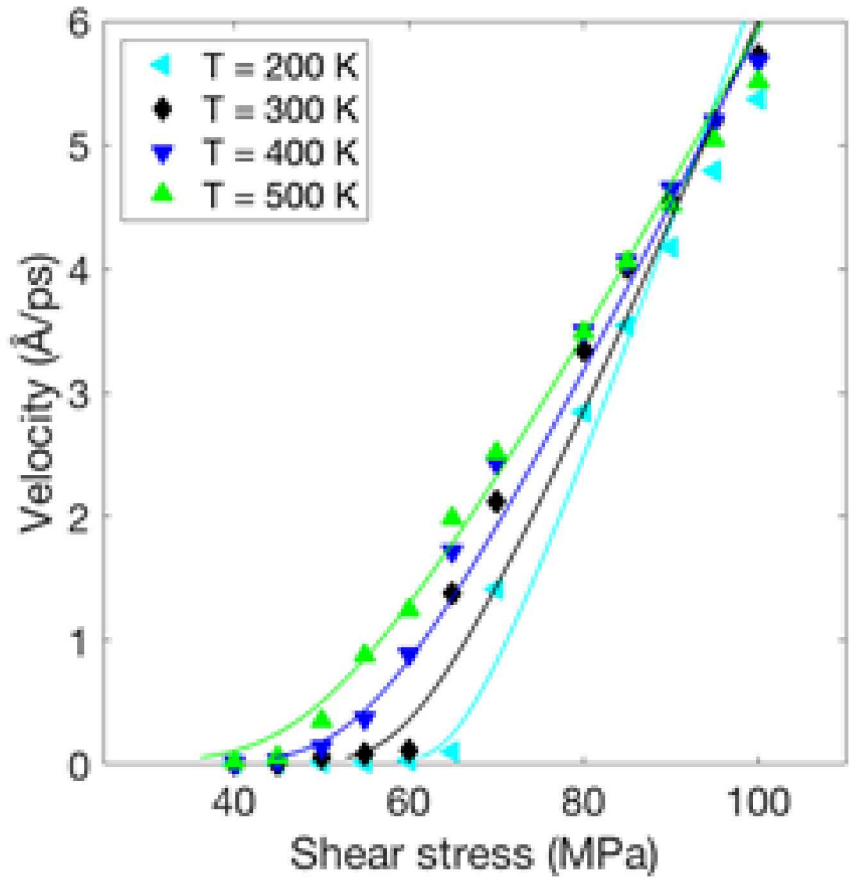
$$v = 2w\omega_H exp\left(-\frac{\Delta E_b}{k_B T}\right) sinh\left(\frac{\Delta E_b}{k_B T}\frac{\tau}{\tau_{y0}}\right)$$

Parameter: ΔE_b, $w\omega_H$, τ_{y0}, C, n, s, c_T, β.

$\tau_{y0} = 77.7$ MPa

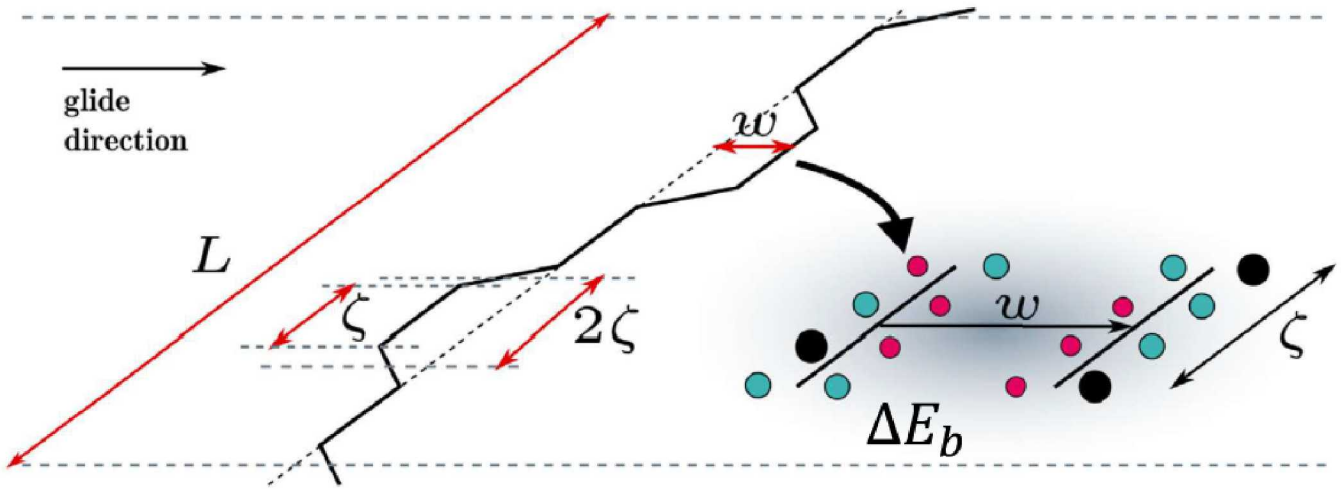
$\Delta E_b = 0.725$ eV

$w\omega_b = 4.35 \times 10^4$ m/s

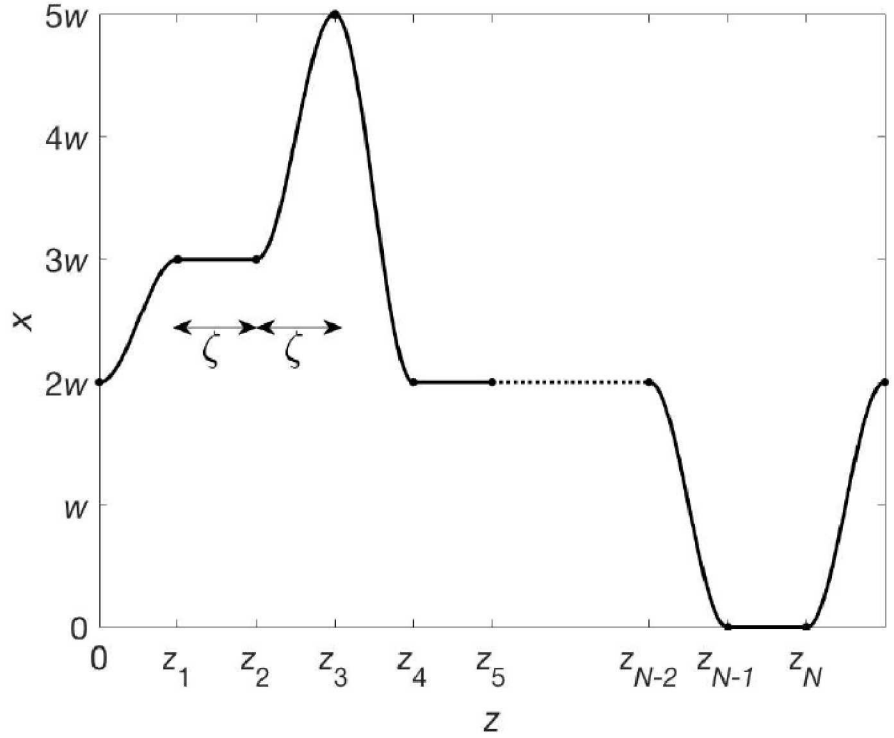


Kinetic Monte Carlo (kMC) Model

Varvenne et al. (2016)



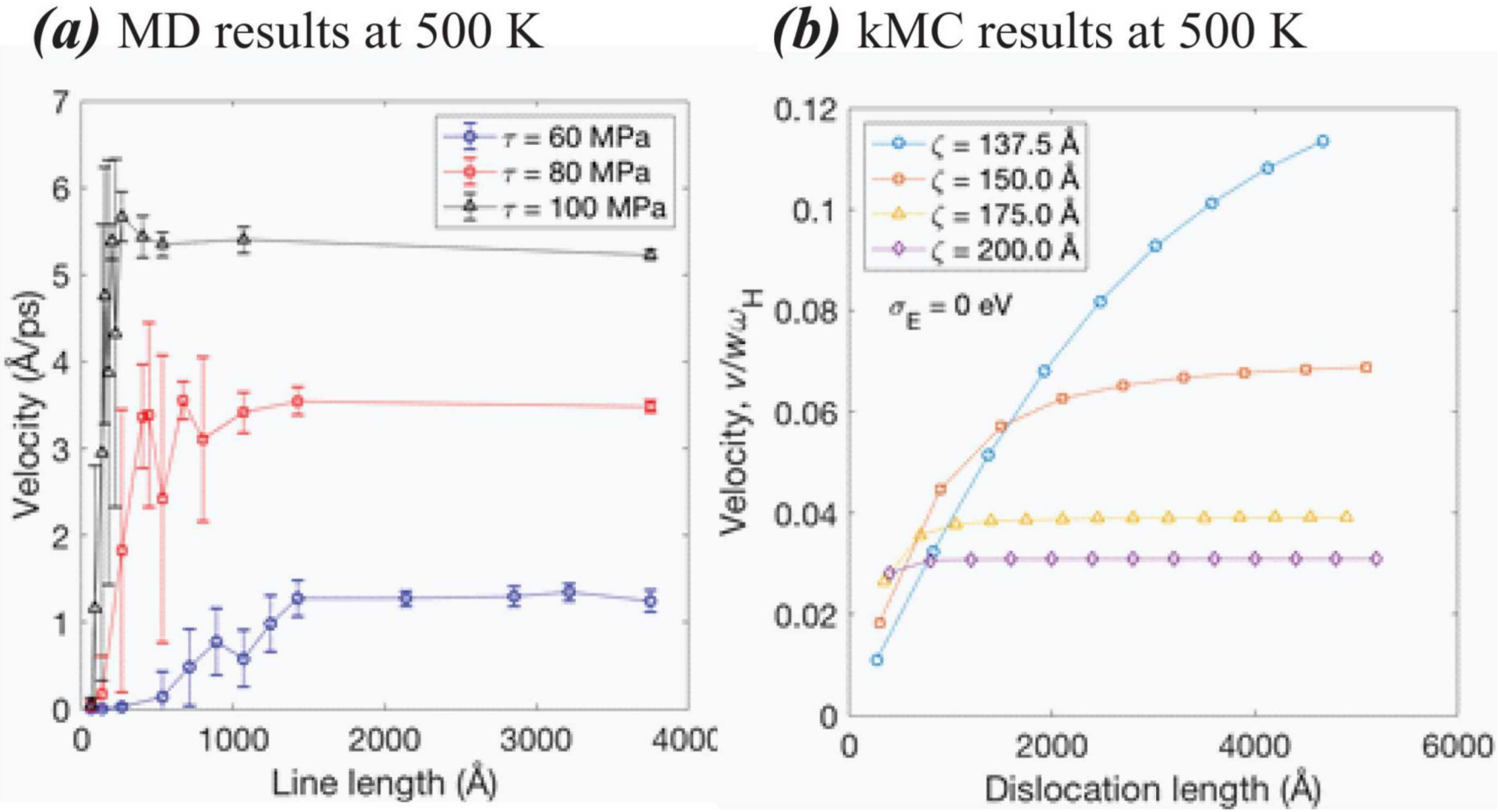
Solid solution strengthening theory of Leyson et al. (2010)



Sinusoidal line profile with discrete "control points"

Dislocation migrates through activation of ζ segments.

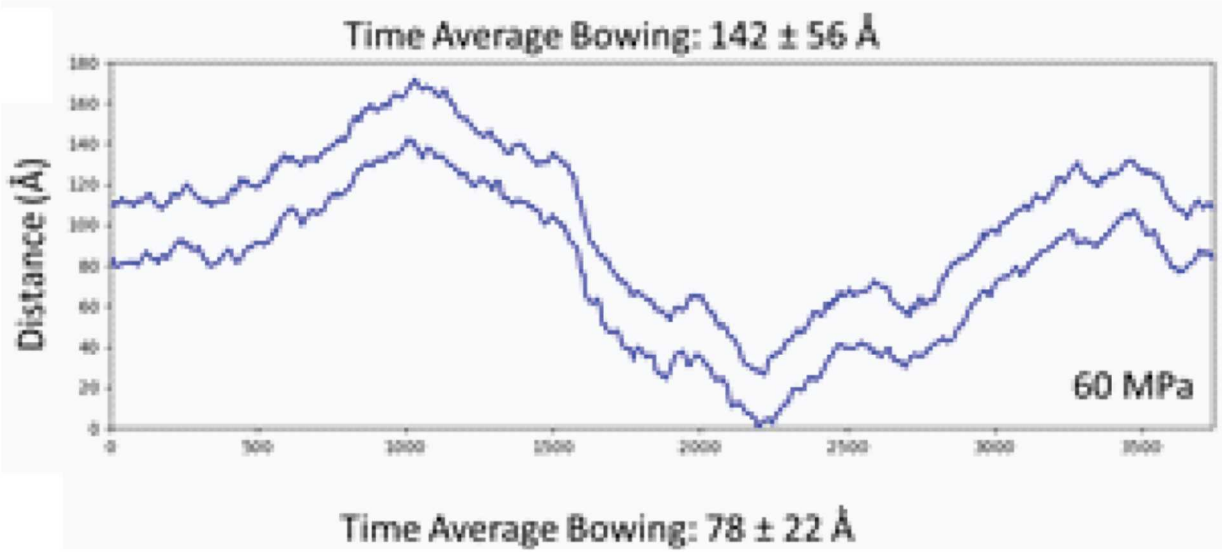
MD vs. Model on Dislocation Velocity



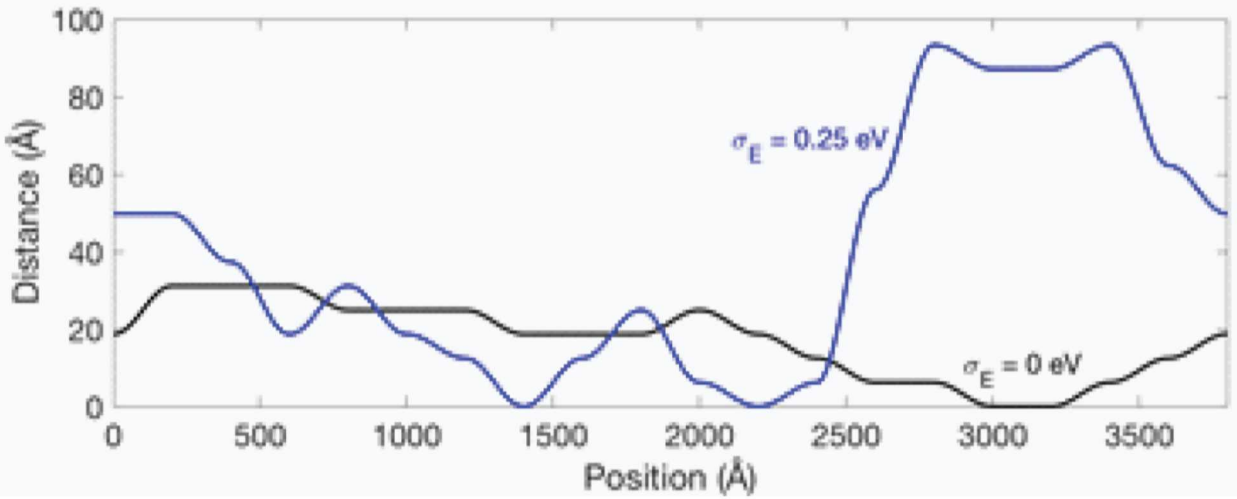
- σ_E: standard deviation of energy barriers of segments ζ.
- Length dependence comes from solute dragging effects.
- Segment length ζ impacts the length dependence.

MD vs. Model on Dislocation Shape

(a) MD results at 500 K, 60 MPa



(b) kMC results at 500 K, 60 MPa, ζ = 200 Å



- σ_E is standard deviation of energy barrier distribution.
- Need a spatially varying energy barrier to reproduce large-scale bowing.

Conclusions

- MD simulations reveal fundamental relationships between stress, temperature, and size.
- Model accounting for solute, phonon, and singular dragging can rationalize MD results.
- kMC results indicate that the size dependence origins from activation of local dislocation segments.
- Energy barrier dislocation impact bowing scale.
- Results stimulate new strengthening ideas to limit activated dislocation length such as nanostructuring and composition modulation etc.