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

SAND2019-14936C

International Conference on Plasticity, Damage & Fracture

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

X. W. Zhou[1], R. B. Sills[2], and M. E. Foster[1]

[1]Sandia National Laboratories, Livermore, California 94550, USA

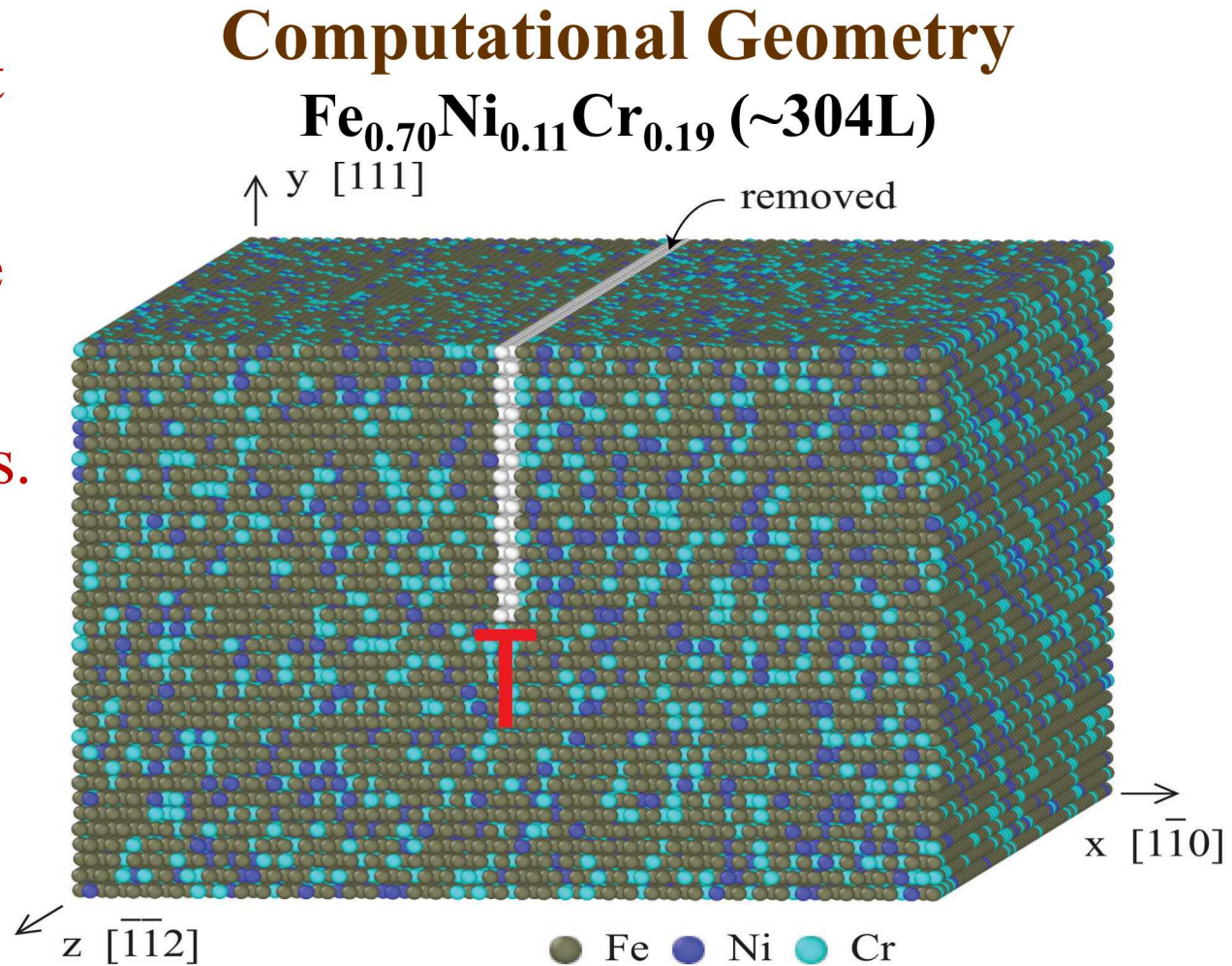[2]Rutgers University, Piscataway, New Jersey 08854, USA

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.

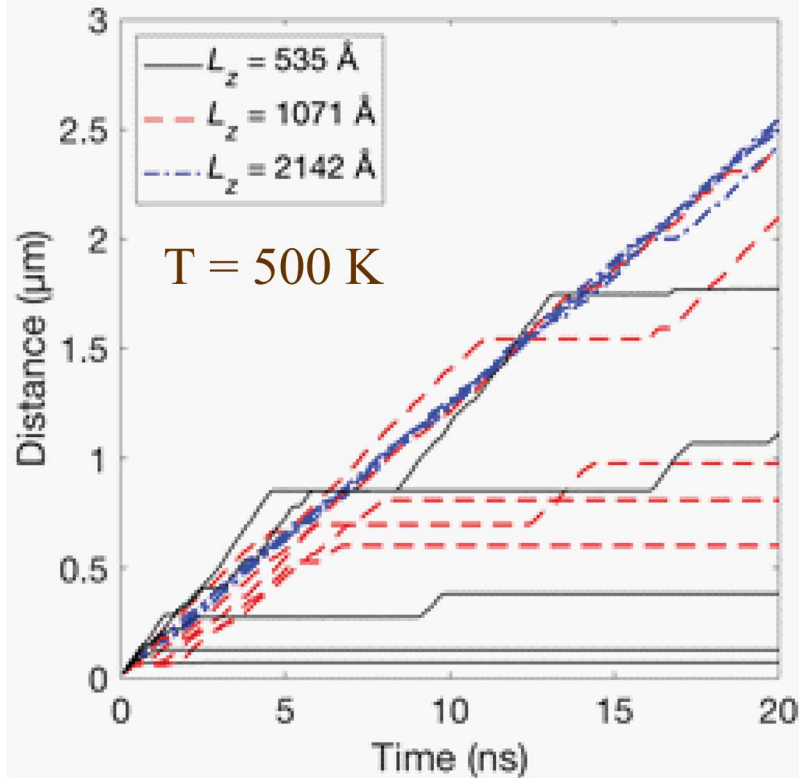❑ Understand when and why the mobility becomes length-dependent.

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.

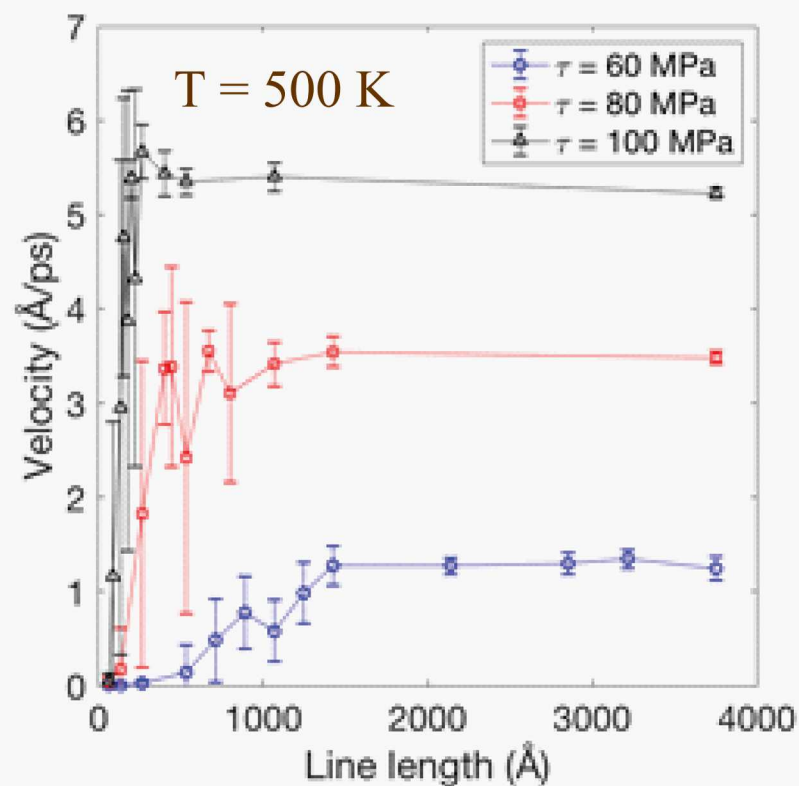- ❑ For each stress / temperature condition, various sizes are explored.

Computational Geometry

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

y [111]

removed

T

x [1$\bar{1}$0]

z [$\bar{1}\bar{1}$2]

● Fe ● Ni ● Cr

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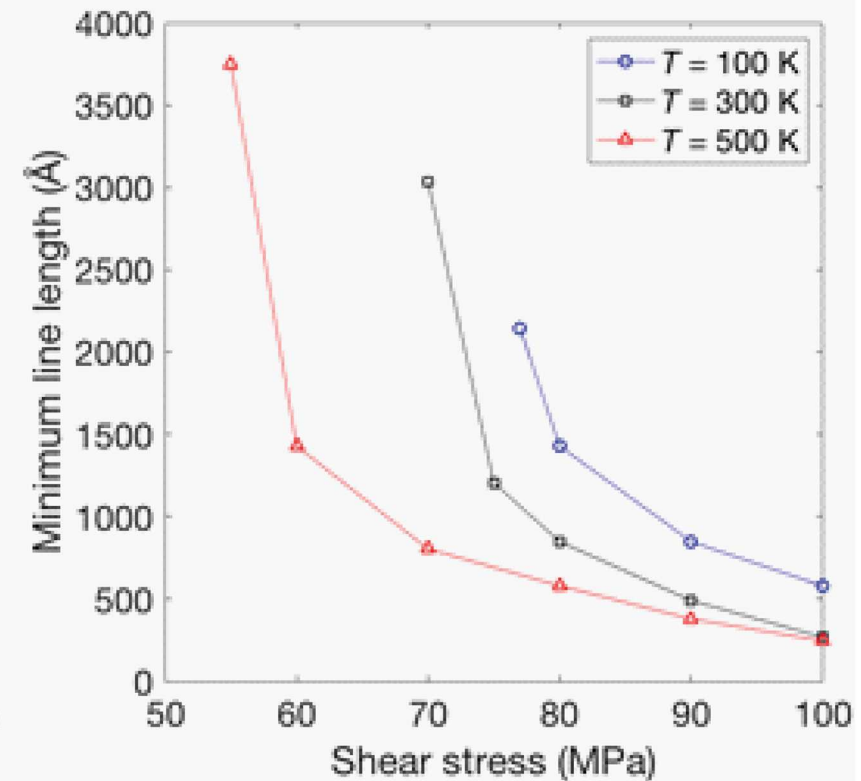
Size Effects

(a) distance at τ = 60 MPa

(b) velocity

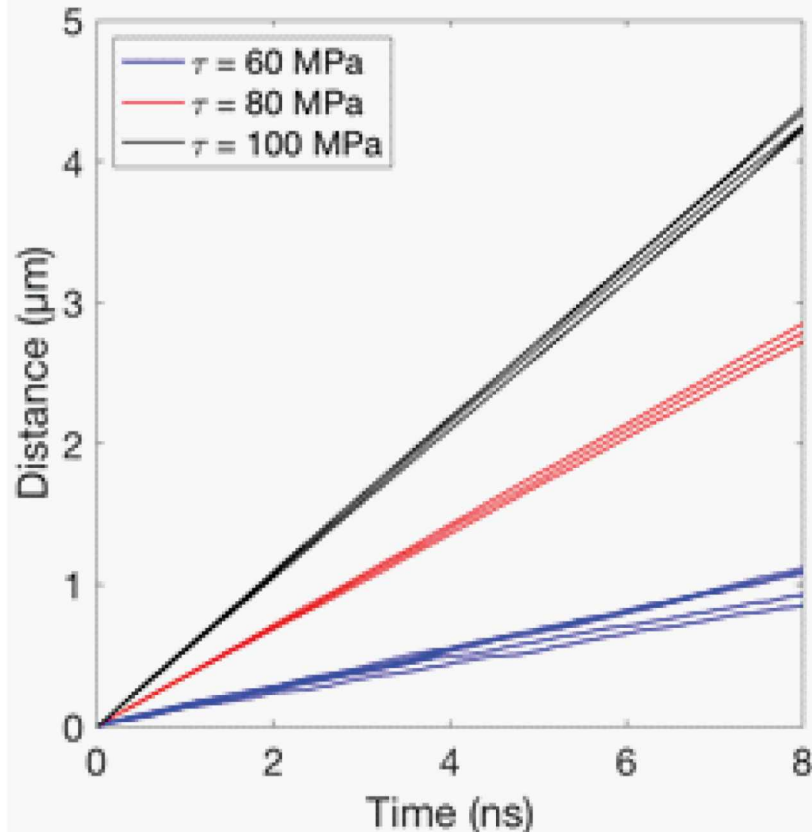**(c)** threshold size-independent length

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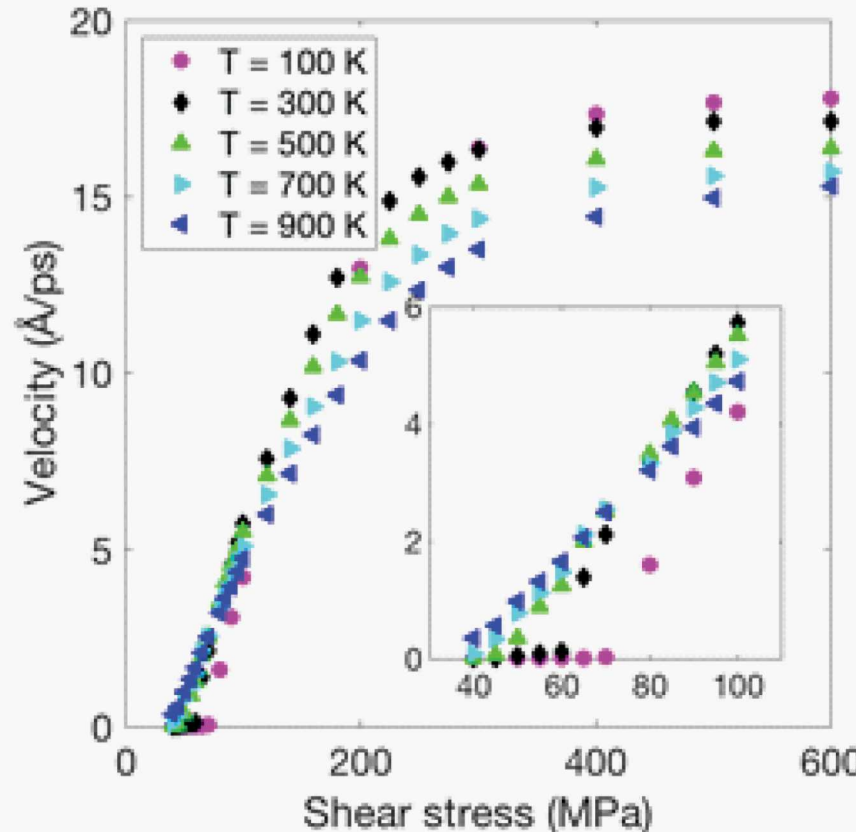❏ **Size-insensitive velocities can be obtained at high stresses and temperatures.**

Selected Dislocation Distance/Velocity

Dislocation length L$_z$ = 3748 Å

(a) distance at T = 500 K

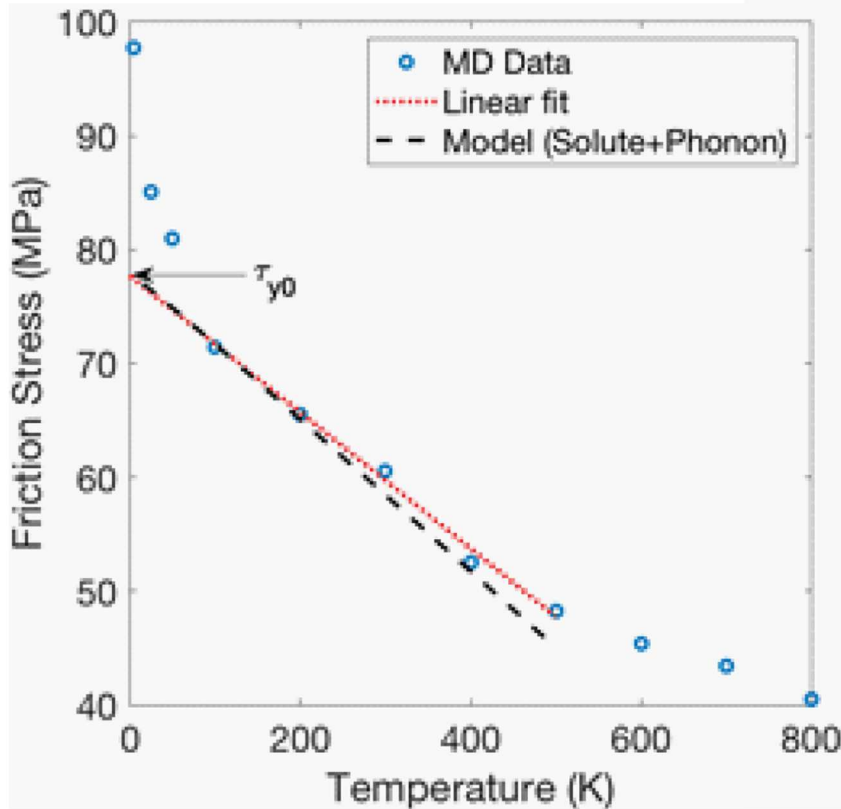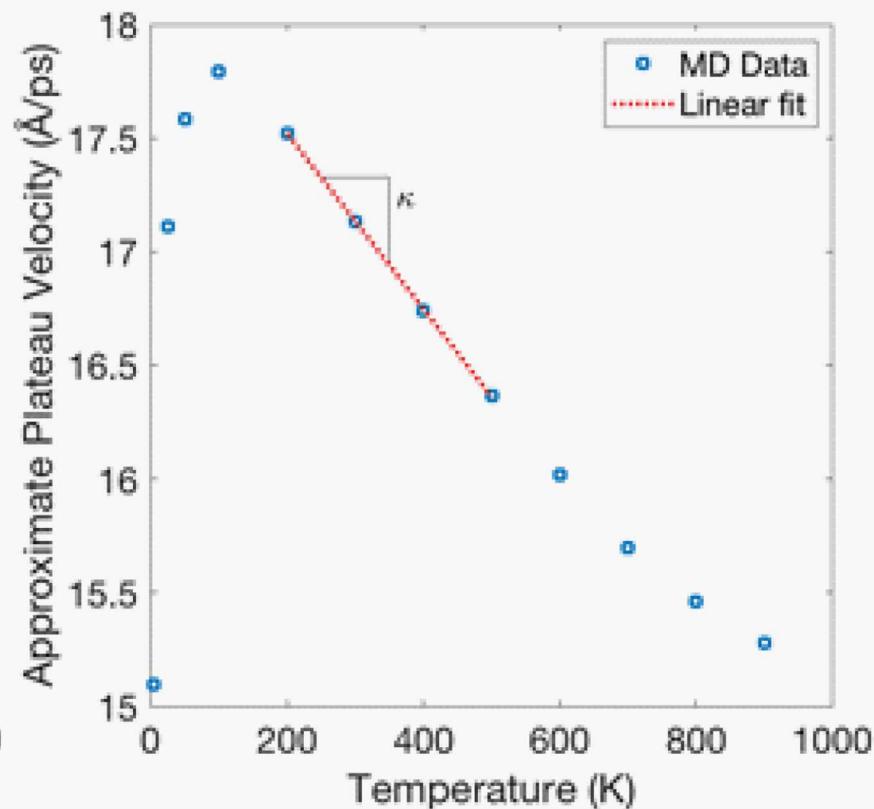*(b)* velocity

- 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 $\tau = 600$ MPa

❑ Friction stress criterion: velocity ≤ 0.25 Å/ps.

❑ At intermediate temperatures, friction stress and plateau velocity both linearly decrease with temperature.

Analytical Mobility Law

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.

$$v = 2w\omega_H exp\left(-\frac{\Delta E_b}{k_B T}\right) sinh\left(\frac{\Delta E_b}{k_B T}\frac{\tau}{\tau_{y0}}\right)$$
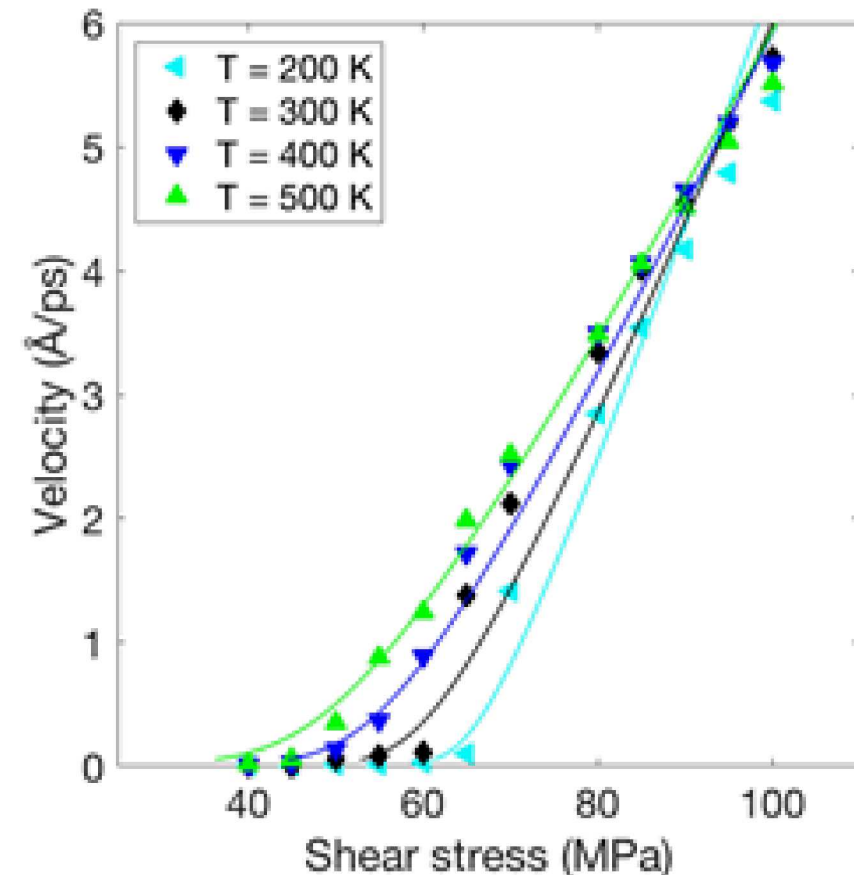
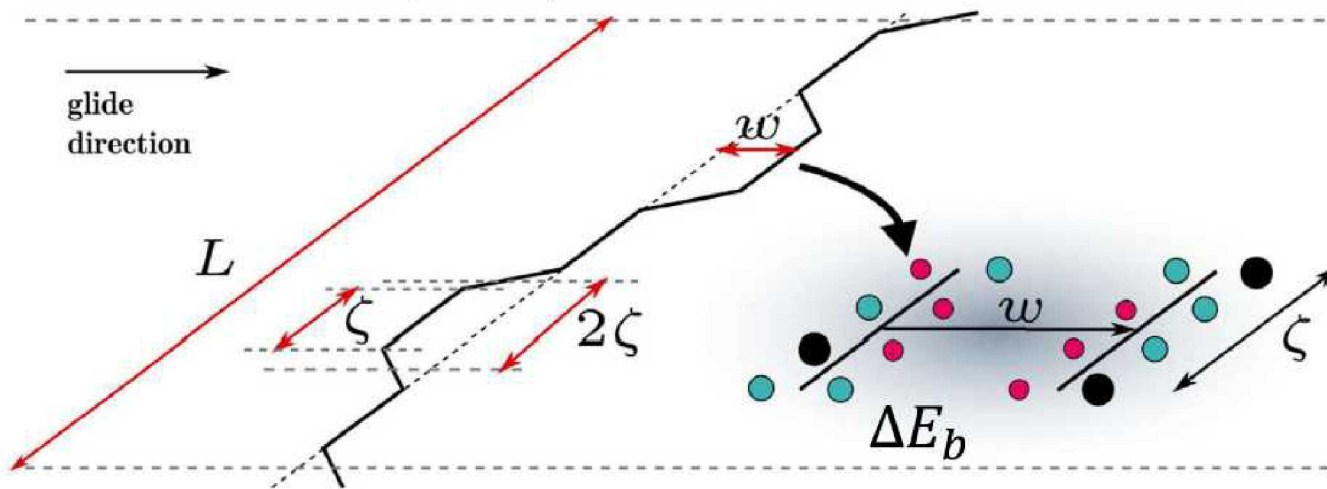**Parameter: ΔE_b, $w\omega_H$, τ_{y0}, C, n, s, c_T, β.**

τ_{y0} = 77.7 MPa
ΔE_b = 0.725 eV
$w\omega_b = 4.35 \times 10^4$ m/s

Kinetic Monte Carlo (kMC) Model

Varvenne et al. (2016)

glide direction

L

ζ

2ζ

w

ΔE_b

w

ζ

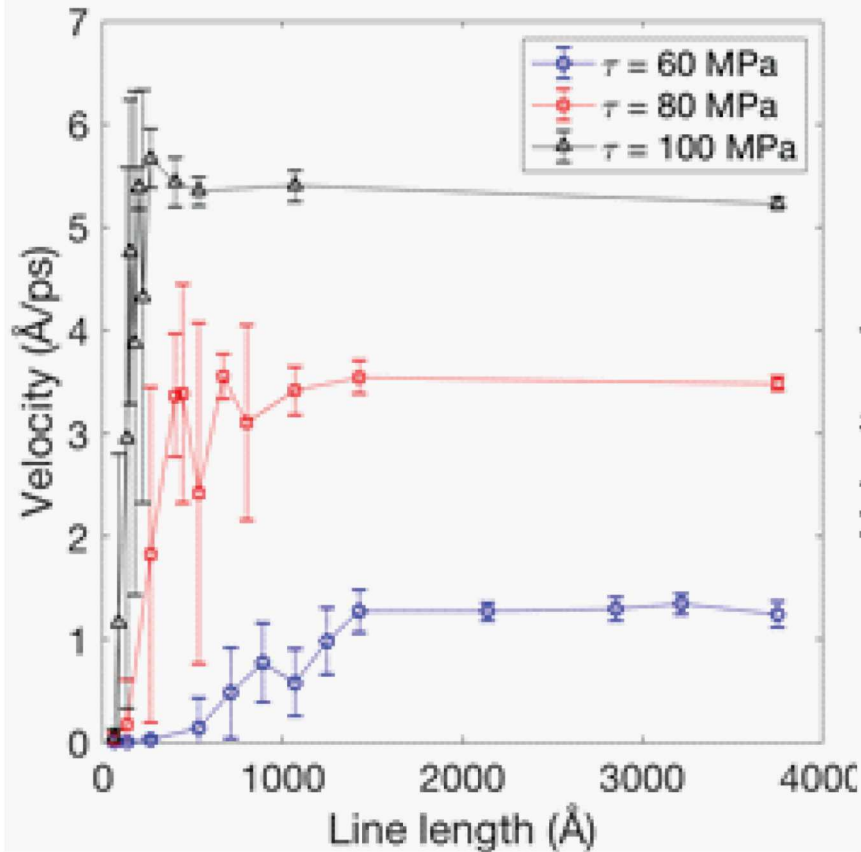Solid solution strengthening theory of
Leyson et al. (2010)

Sinusoidal line profile with discrete
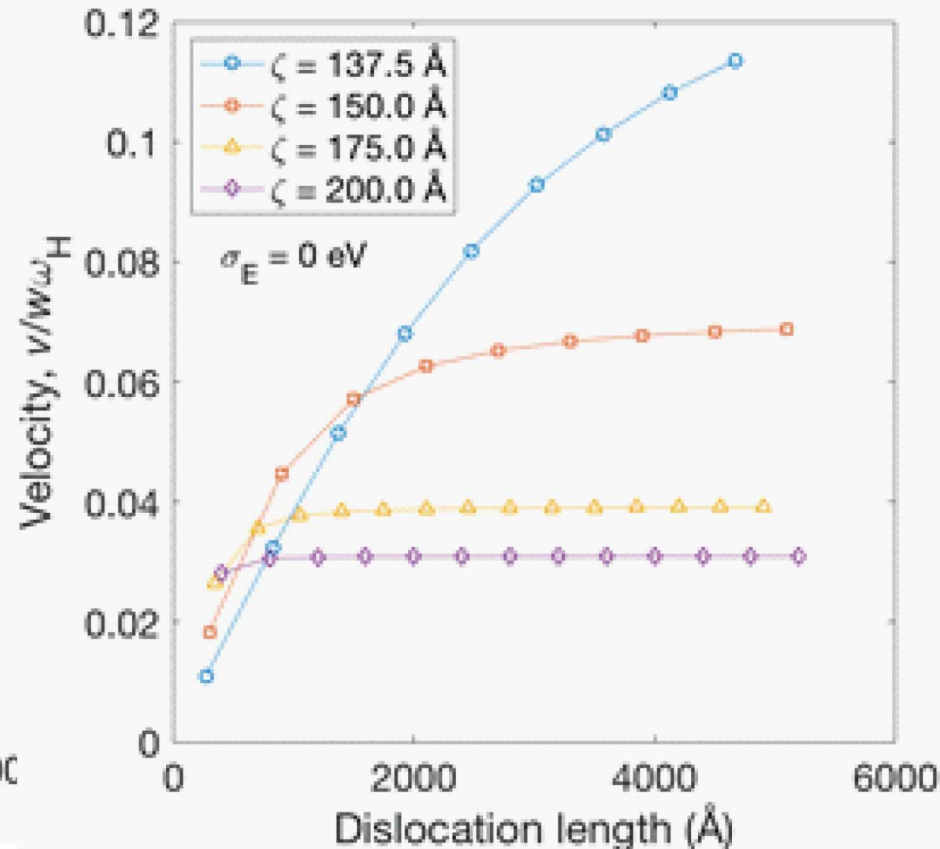"control points"

Dislocation migrates through activation of ζ segments.

MD vs. Model on Dislocation Velocity
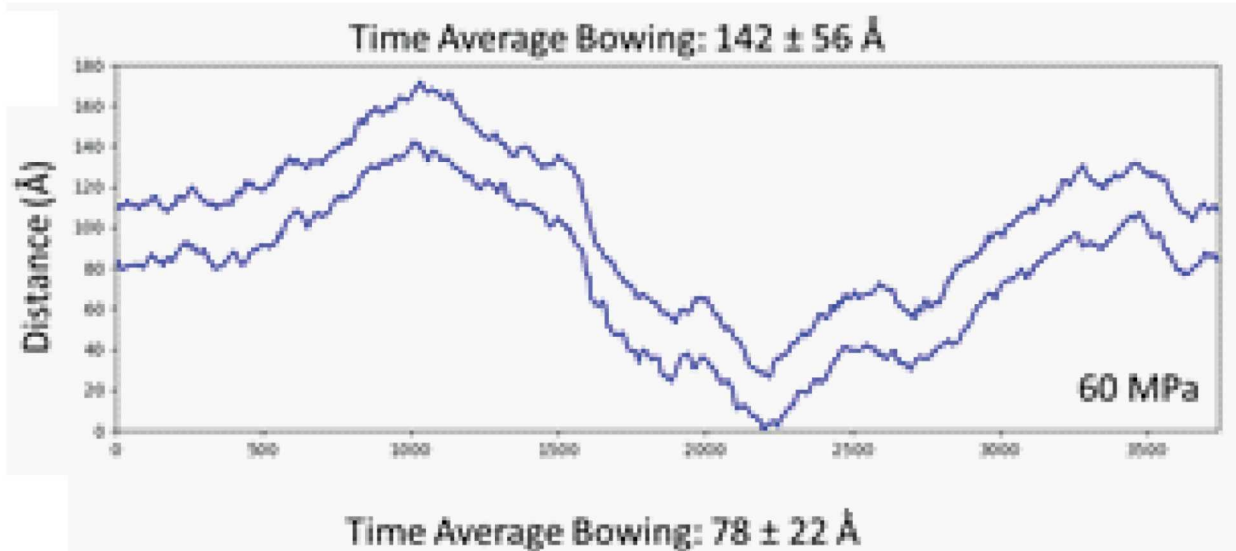
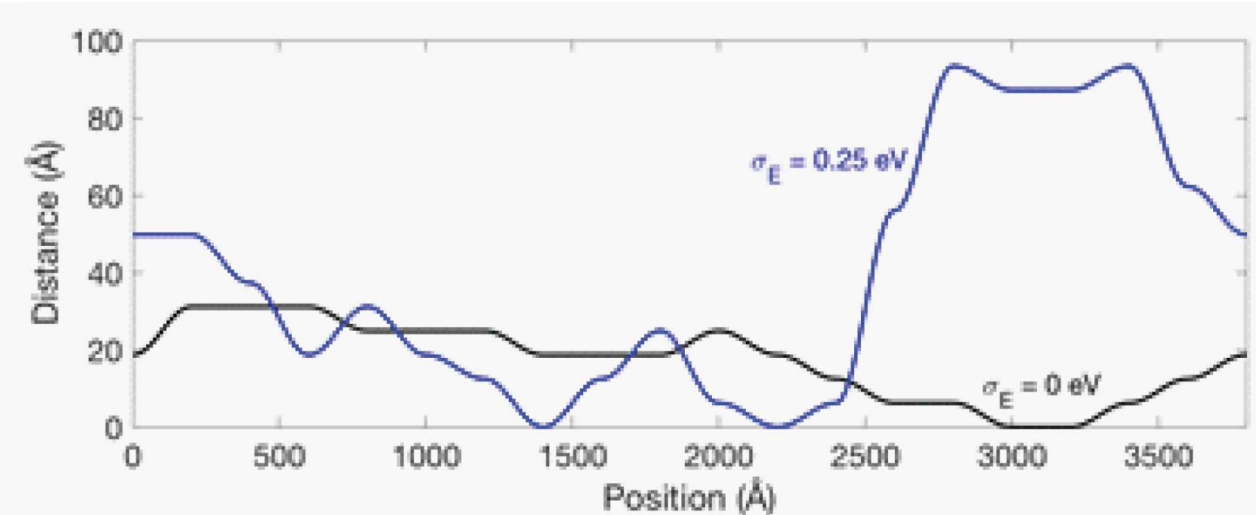**(a)** MD results at 500 K

(b) kMC results at 500 K

- ❑ 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, $\zeta = 200$ 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.