ATOMISTIC APPROACHES FOR CONSTRUCTION OF CONTINUUM DISLOCATION PLASTICITY MODEL

Alexander Mayer, Vasiliy Krasnikov and Victor Pogorelko

Chelyabinsk State University, Chelyabinsk, Russia
mayer@csu.ru

Copper plate after high-current electron irradiation

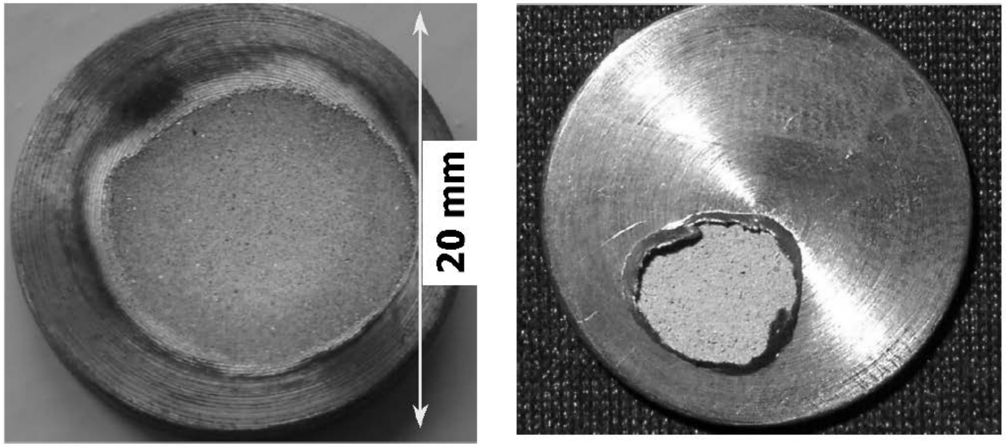


Fig. 3. Front (left) and rear (right) specimen surfaces upon a one-pass electron beam treatment

Markov A.B., et al. // 7-th Int. Conf. Modification of Materials with Particle Beams and Plasma Flows. Proc. Tomsk: IHCE SB RAS. (2004)

D16 aluminum alloy after high-velocity impact

Mescheryakov Yu.I., Divakov A.K., In: Shock Compression of Condensed Matter-2003; AIP Proc. (2004)

Ultra-fast laser generated shocks in thin films

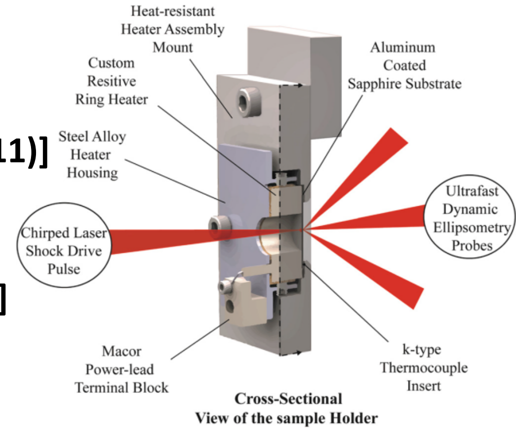
Al – [Ashitkov S.I., Agranat M.B., Kanel' G.I., Komarov P.S., Fortov V.E., JETP Lett. (2010)]

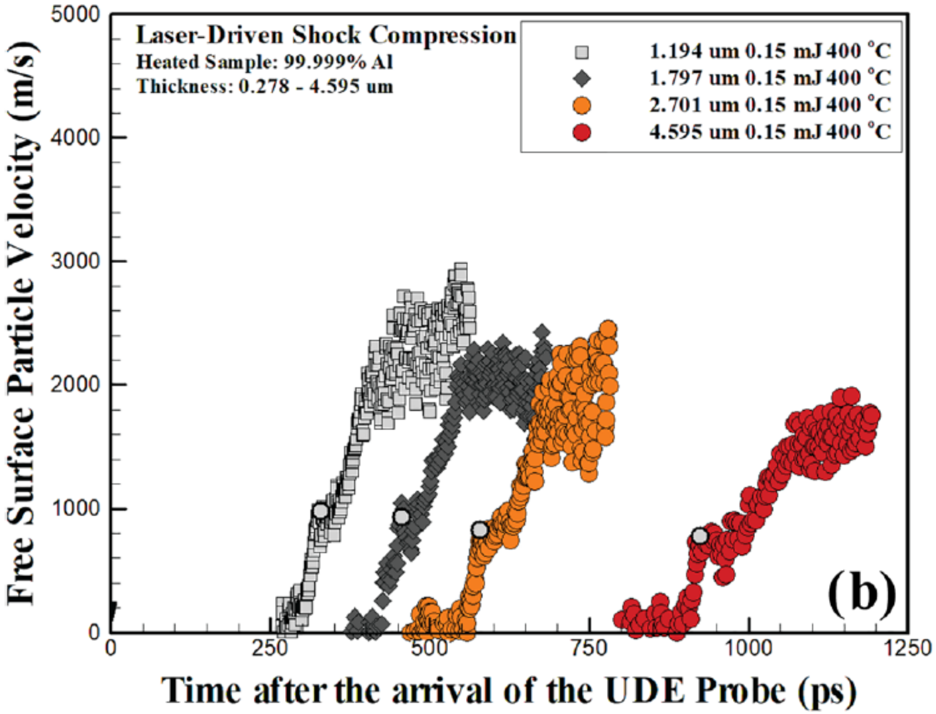
Al – [Whitley V., McGrane S., Eakins D., Bolme C., Moore D., Bingert J., J. Appl. Phys. (2011)]

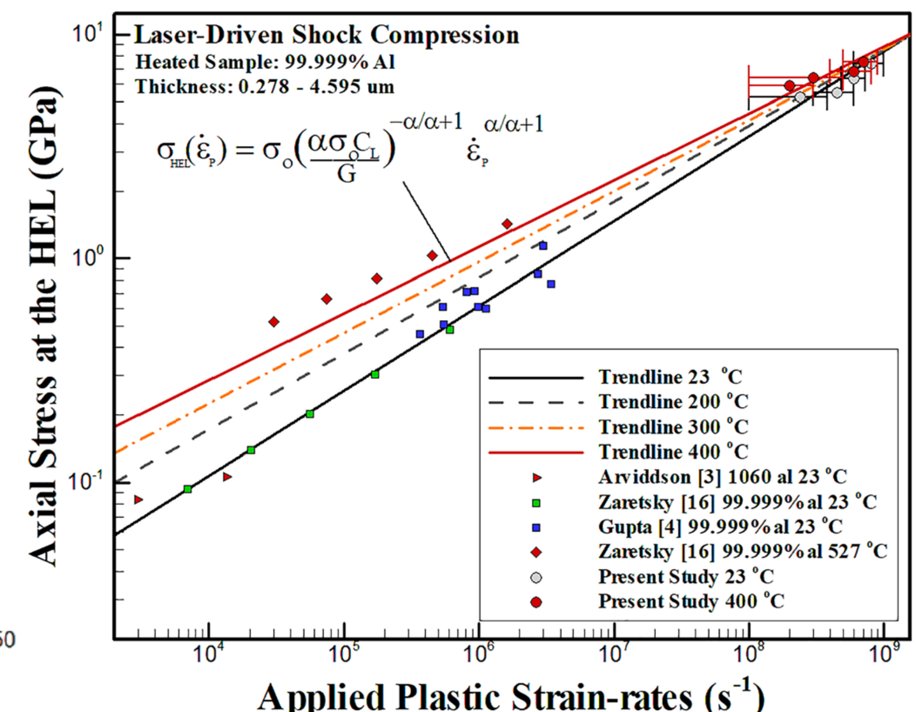
Fe – [Ashitko S.I., Komarov P.S., Agranat M.B., Kanel G.I., Fortov V.E., JETP Lett. (2013)]

V – [Ashitkov S.I., Komarov P.S., Struleva E.V., Agranat M.B., Kanel G.I., JETP Lett. (2015)]

Al – [Zuanetti B., McGrane Sh.D., Bolme C.A., Prakash V., J. Appl. Phys. (2018)]







Continuum mechanics

$$\dot{\rho} = -\rho\left[\left(\nabla\cdot\mathbf{v}\right)+\dot{W}\right]$$ equation of continuity

$$\dot{\mathbf{v}} = \frac{1}{\rho}\left[-\left(\nabla P\right)+\left(\nabla\cdot\mathbf{S}\right)-P\left(\nabla W\right)-\left(S\cdot\nabla\right)W\right]$$ equation of motion

$$\dot{E} = \frac{1}{\rho}\left[-P\left(\left(\nabla\cdot\mathbf{v}\right)+\dot{W}\right)+\left(\mathbf{S}:\dot{\mathbf{w}}\right)\right]+D-\left(\nabla\cdot\mathbf{q}\right)$$ equation for internal energy

$$\boldsymbol{\sigma} = -P\cdot\mathbf{I}+\mathbf{S}$$ stresses

$$P = P\left(\rho,E\right) \quad T = T\left(\rho,E\right)$$ equation of state (EOS)

Plasticity model (dislocations)

$\mathbf{w}$ plastic deformation tensor

$\mathbf{S}$ stress deviator

Fracture model

$\mathbf{W}$ material deformation at the expense of formation and growth of damages

$$W = \mathrm{trace}(\mathbf{W})$$

Dislocation plasticity model

Generalized Hooke law

$$\mathbf{S} = 2G\left[\mathbf{u} - \frac{u}{3}\mathbf{I} - \mathbf{w}\right] \qquad u = \mathrm{trace}(\mathbf{u})$$

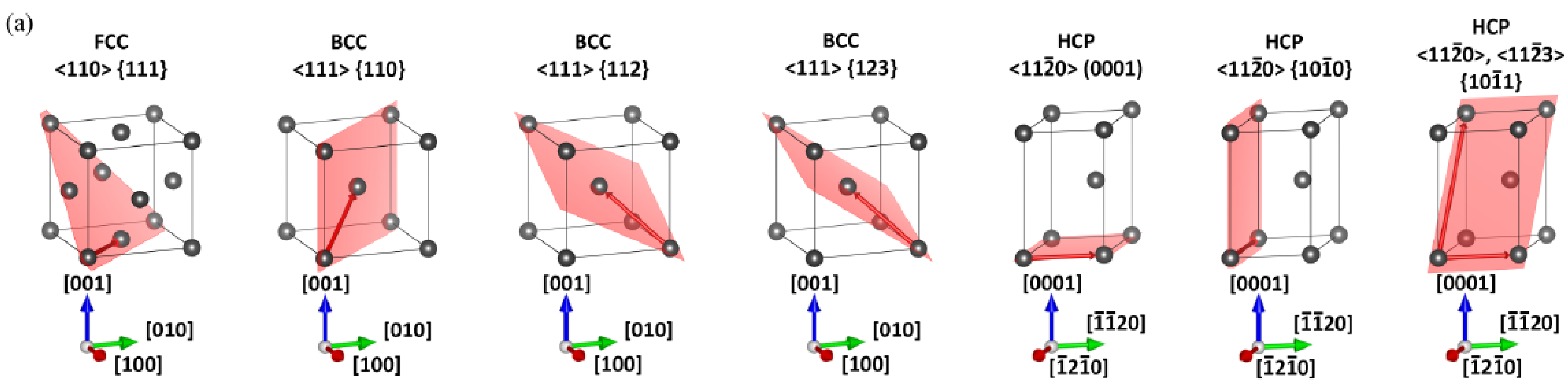
Macroscopic deformation

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathrm{sym}(\nabla \cdot \mathbf{v}) + \mathrm{rotation}$$

Dislocation slip

$$\frac{\mathrm{d}\mathbf{w}}{\mathrm{d}t} = \frac{1}{2}\sum_{\beta} \mathrm{sym}\left(\mathbf{b}^{\beta} \otimes \mathbf{n}^{\beta}\right) V_D^{\beta}\, \rho_D^{\beta} + \mathrm{rotation}$$

$\mathbf{b}^{\beta}$ - Burgers vector; $\mathbf{n}^{\beta}$ - normal to the slip plane



[Kwa´sniak P., ´Spiewak P., Garbacz H., Kurzydłowski K.J., Phys. Rev. B (2014)]

Motion of dislocations in pure metals

$$m_0 \frac{\mathrm{d}V_{\mathrm{D}}^{\beta}}{\mathrm{d}t} = \left[\left(\mathbf{b}^{\beta} \cdot \mathbf{S} \cdot \mathbf{n}^{\beta} \right) - \frac{1}{2} bY \,\mathrm{sign}\left(V_{\mathrm{D}}^{\beta} \right) \right] \left[1 - \left(V_{D}^{\beta} / c_{\mathrm{t}} \right)^2 \right]^{3/2} - BV_{\mathrm{D}}^{\beta}$$

$m_0 \approx \rho^2 b \approx 10^{-16}$ kg/m - rest mass of dislocations

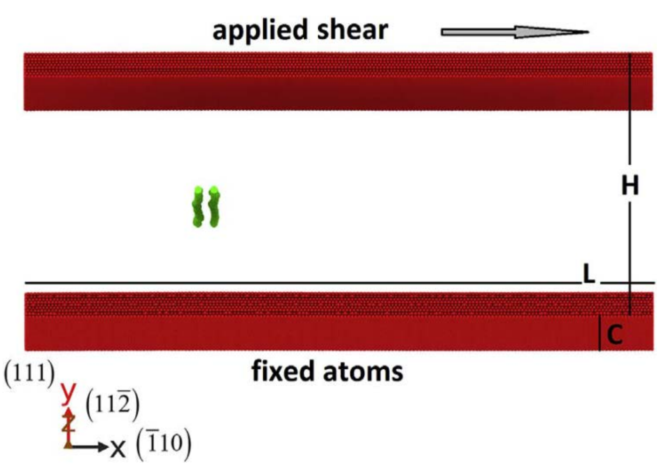
c_{t} - transverse sound velocity

Y - static yield stress

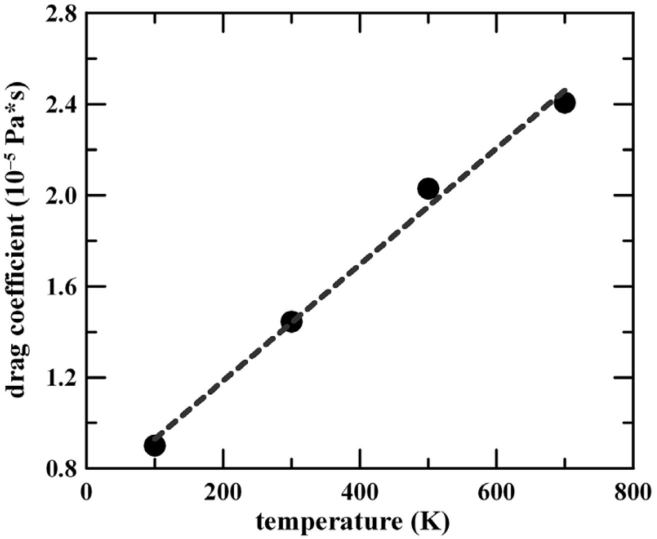
B - drag coefficient

Parameters from MD simulations

[Krasnikov V.S., Mayer A.E., Int. J. Plast. (2018)]

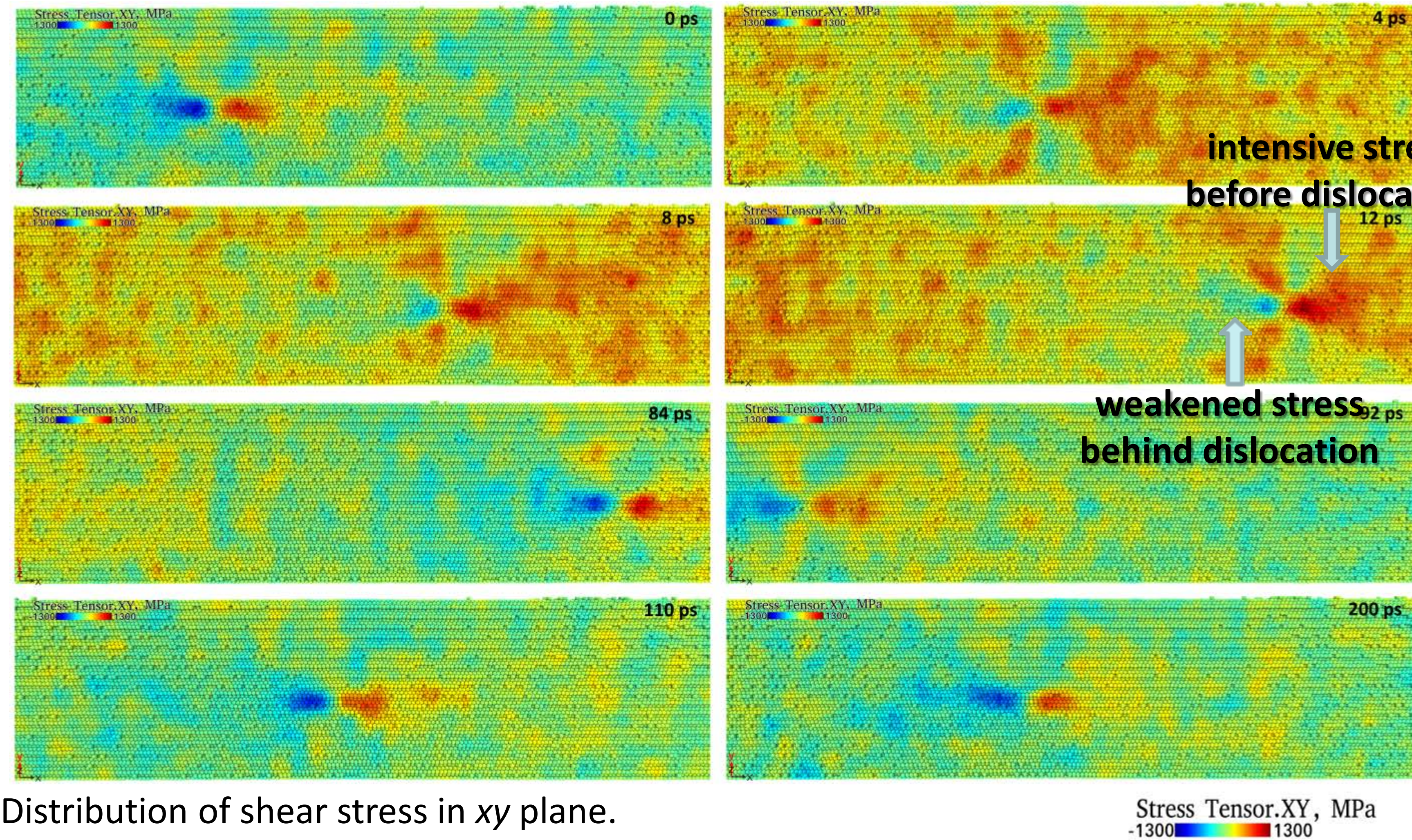


Al



Stress field in Al with moving dislocation

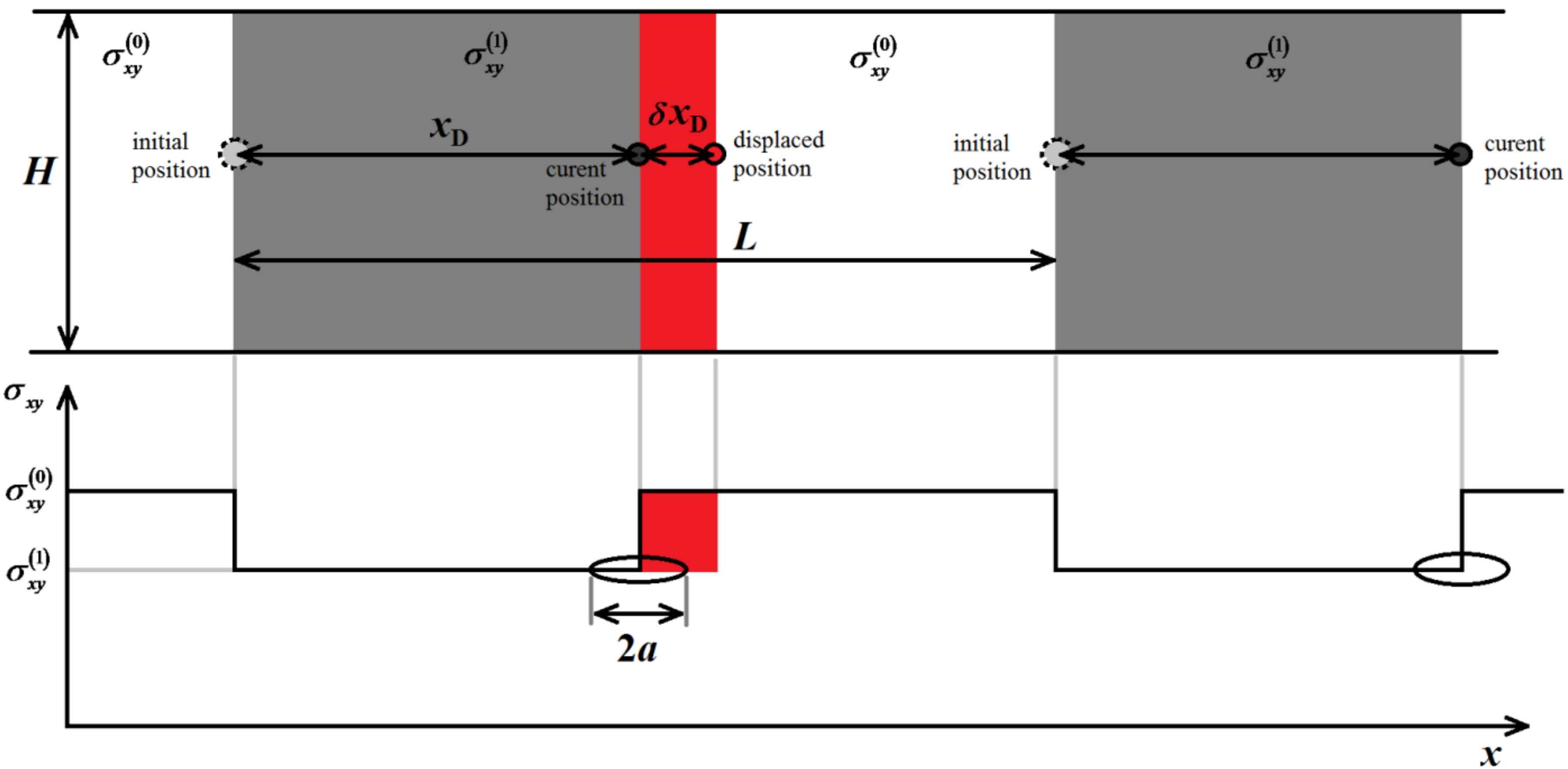
symmetrical initial
stress field of dislocation



Distribution of shear stress in *xy* plane.
Initial displacement *u* is 0.96 nm. Temperature is 300 K.

[Krasnikov V.S., Mayer A.E., Int. J. Plast. (2018)]

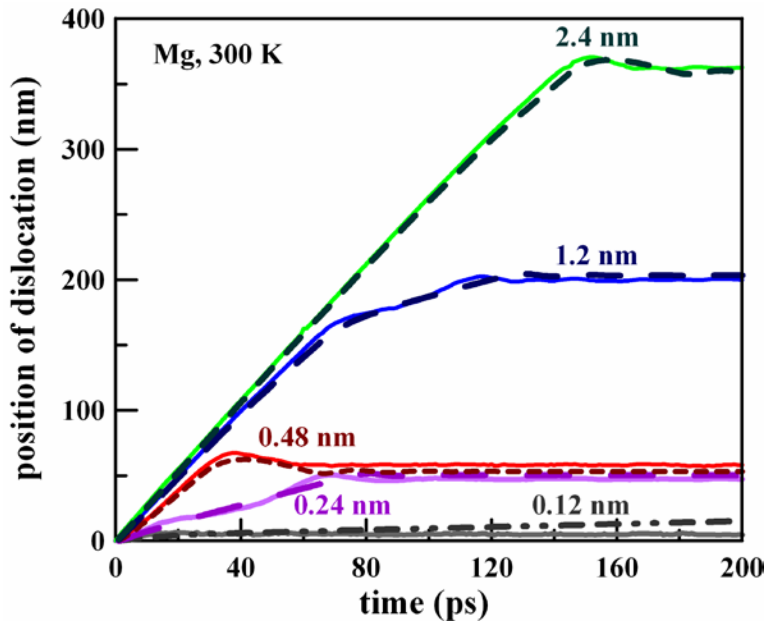
Schema of dislocation motion and stress relaxation

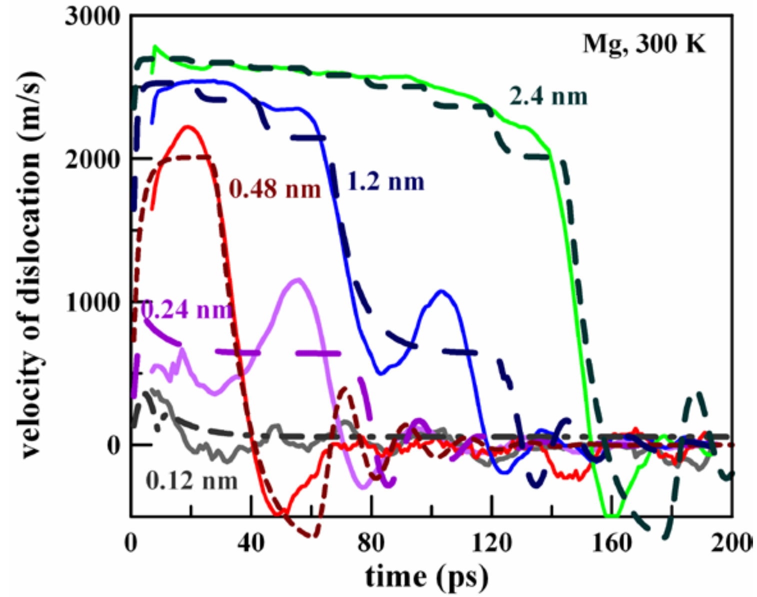


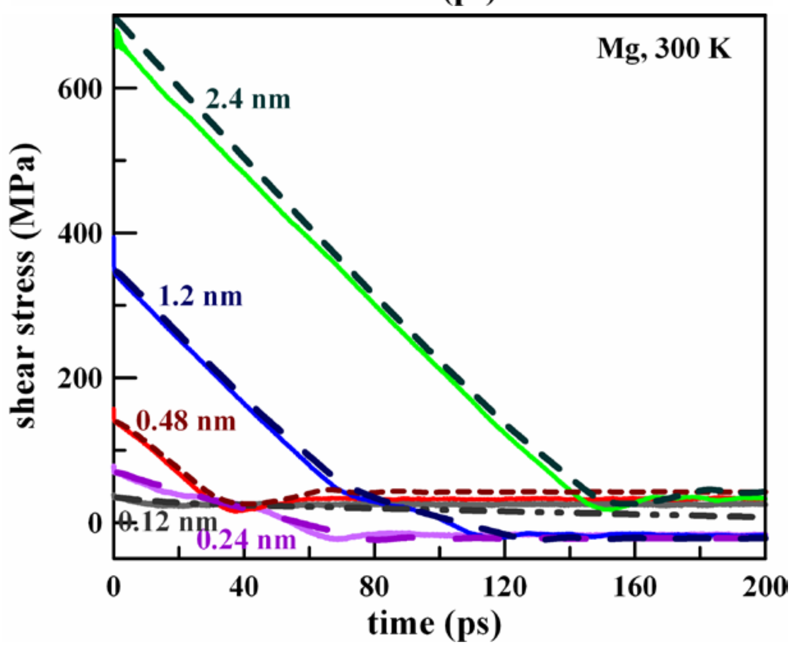
[Krasnikov V.S., Mayer A.E., Int. J. Plast. (2018)]

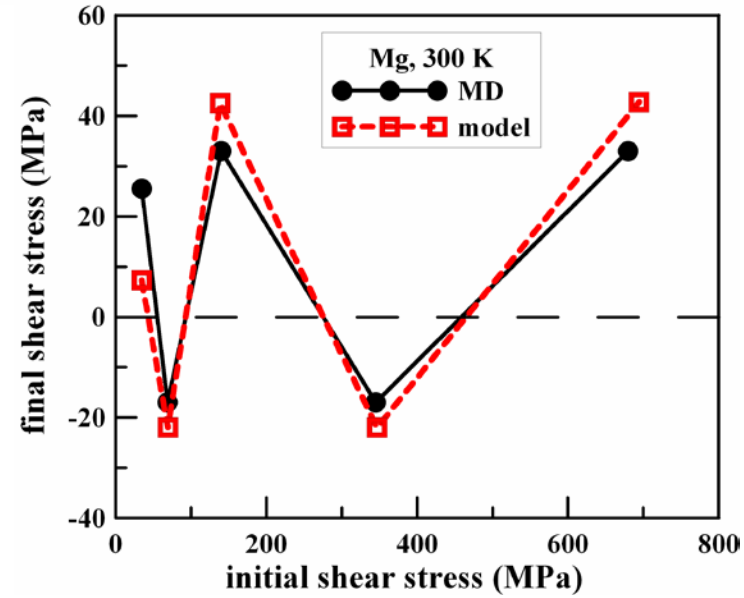
Comparison with MD for Mg

solid lines – MD
dashed lines –dislocation motion equation

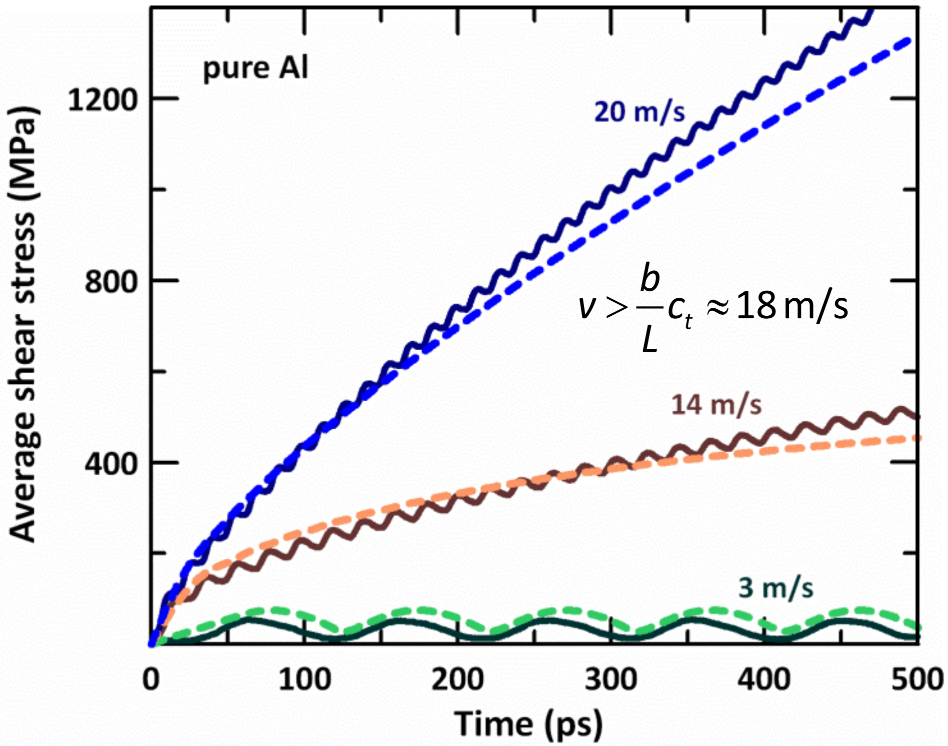


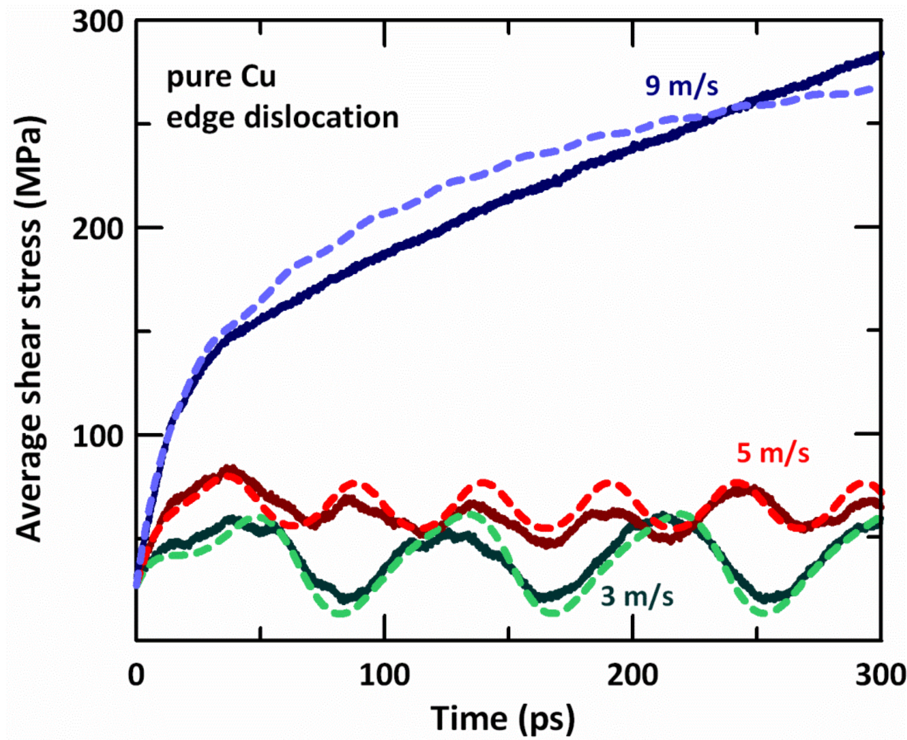




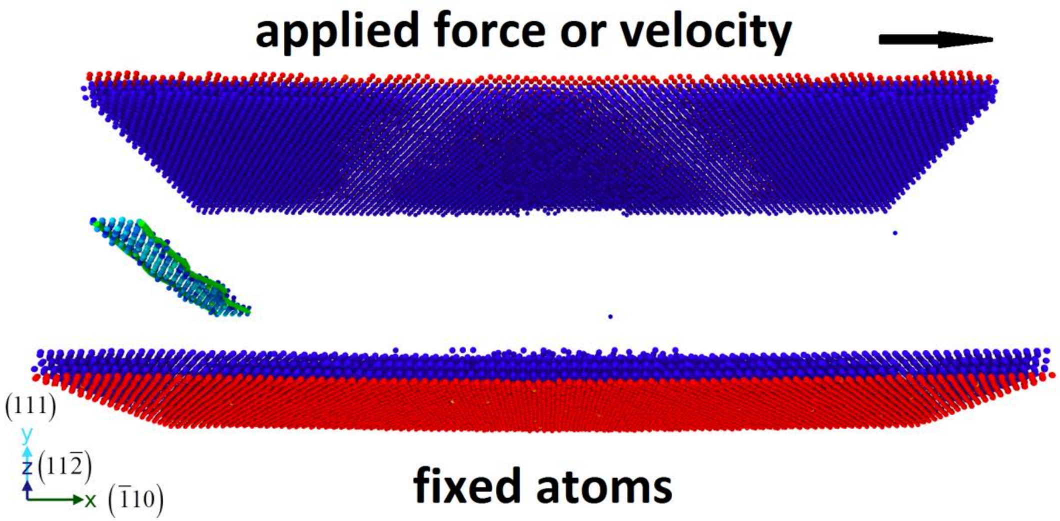


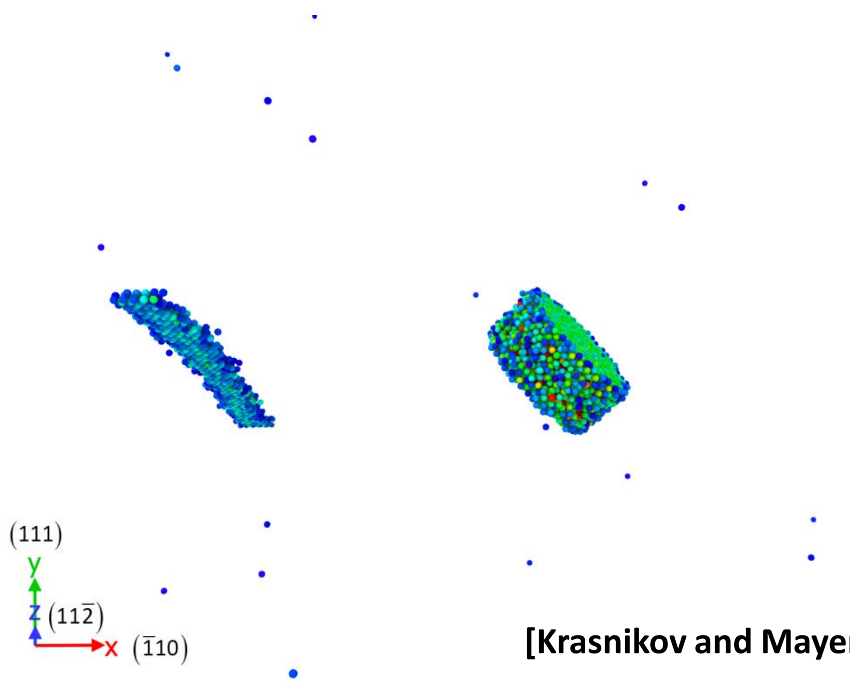
Motion of dislocation at constant rate of shearing





Motion of dislocations in aluminum containing θ‘ phase





θ‘ phase (Al_2Cu).

θ‘ lies on (100) planes.
Dislocation slip plane is (111).
Perfect Burgers vector is oriented along [-110] direction

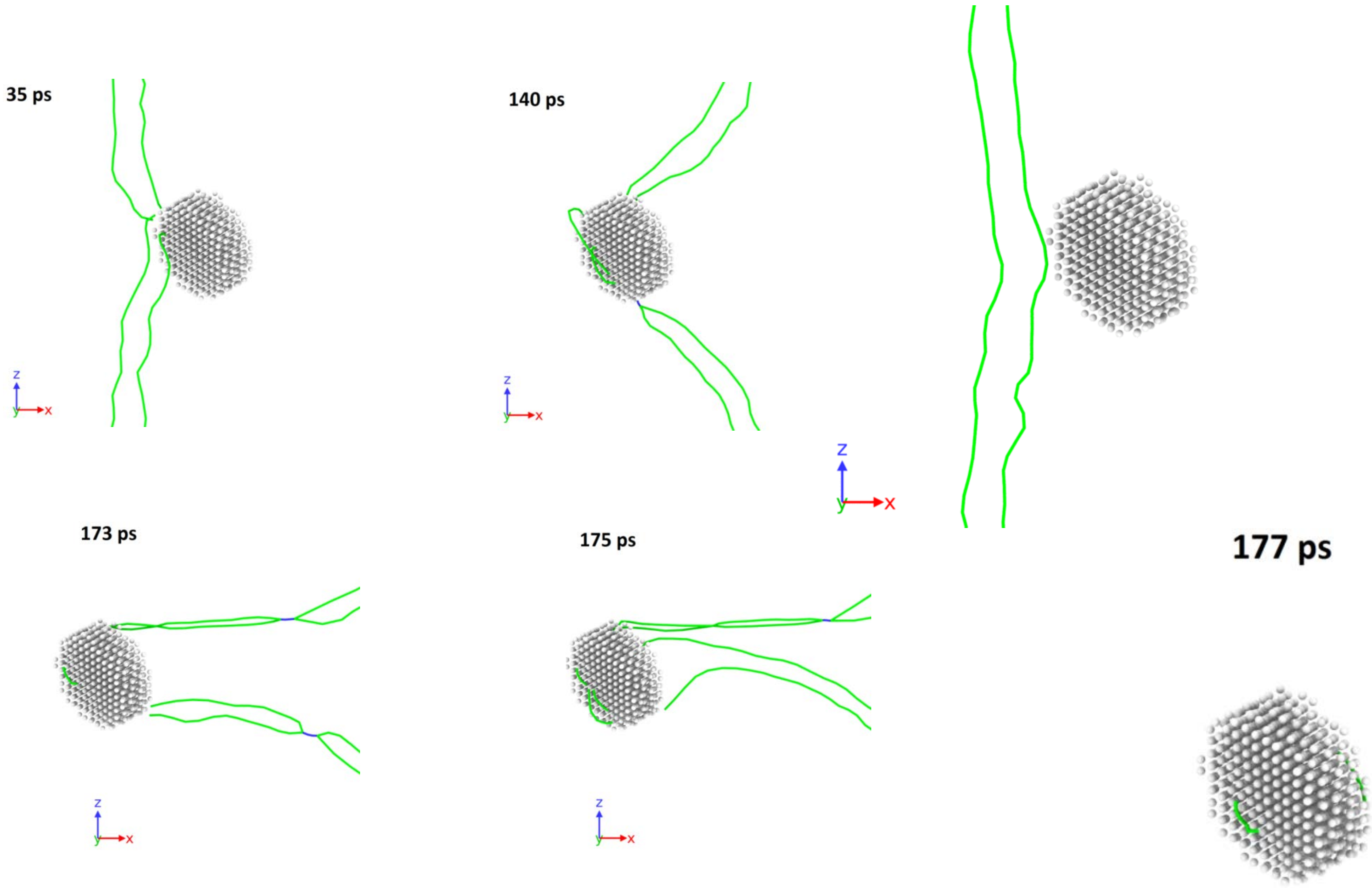
Orientation of calculation area is in accordance with slip system of FCC
[Singh C.V., Warner D.H., Acta Mater. (2010)]

Angle dependent interatomic potential by
[Apostol F., Mishin Y., Phys. Rev. B (2011)]

MD calculations are performed with LAMMPS
[Plimpton S., J. Compute. Phys. (1995)]

[Krasnikov and Mayer, Int. J. Plast. (2019)]

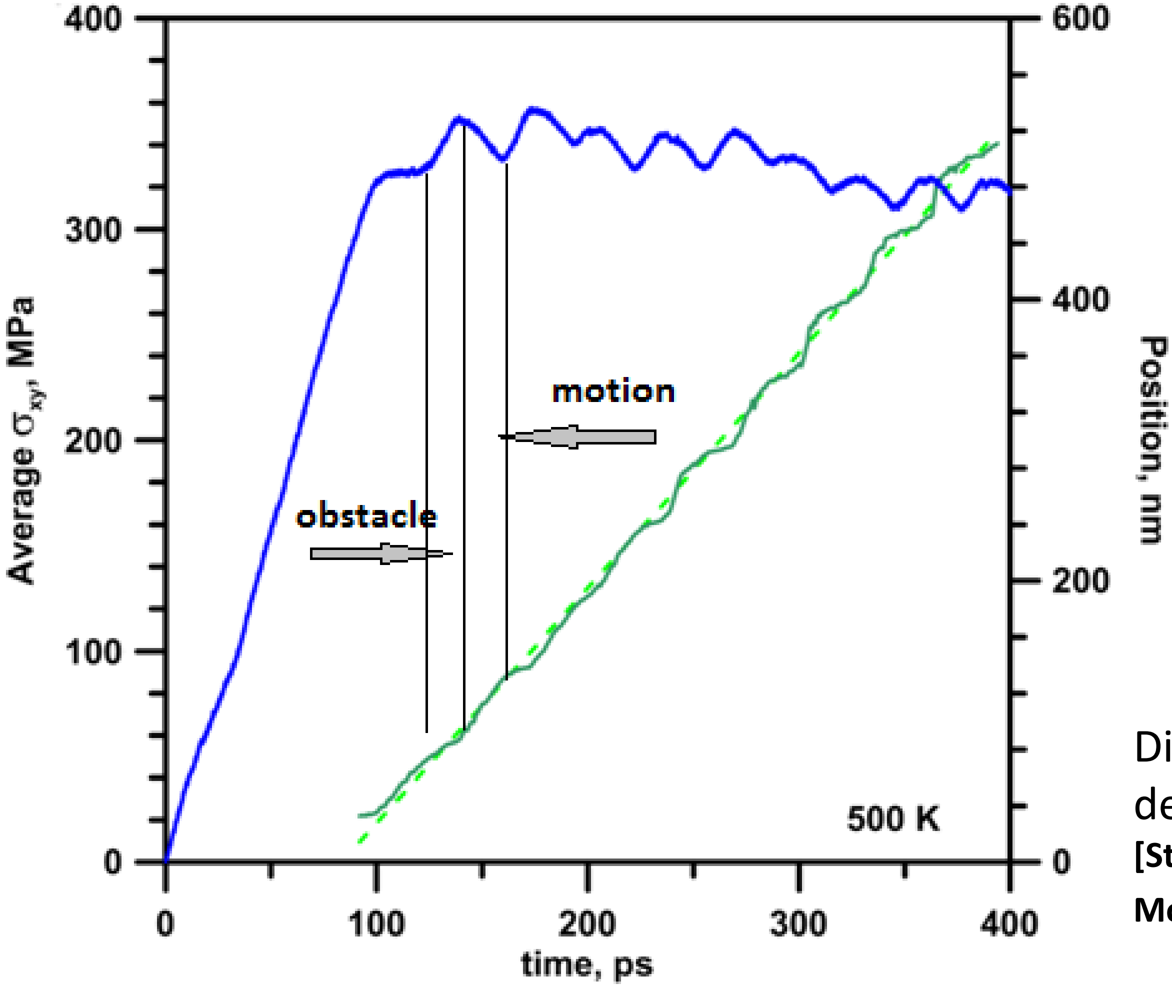
Overcoming of obstacle by dislocation



[Krasnikov and Mayer, Int. J. Plast. (2019)]

Final state with dislocation loop around inclusion

Average stress and position of dislocation



Dislocation position is determined with DXA

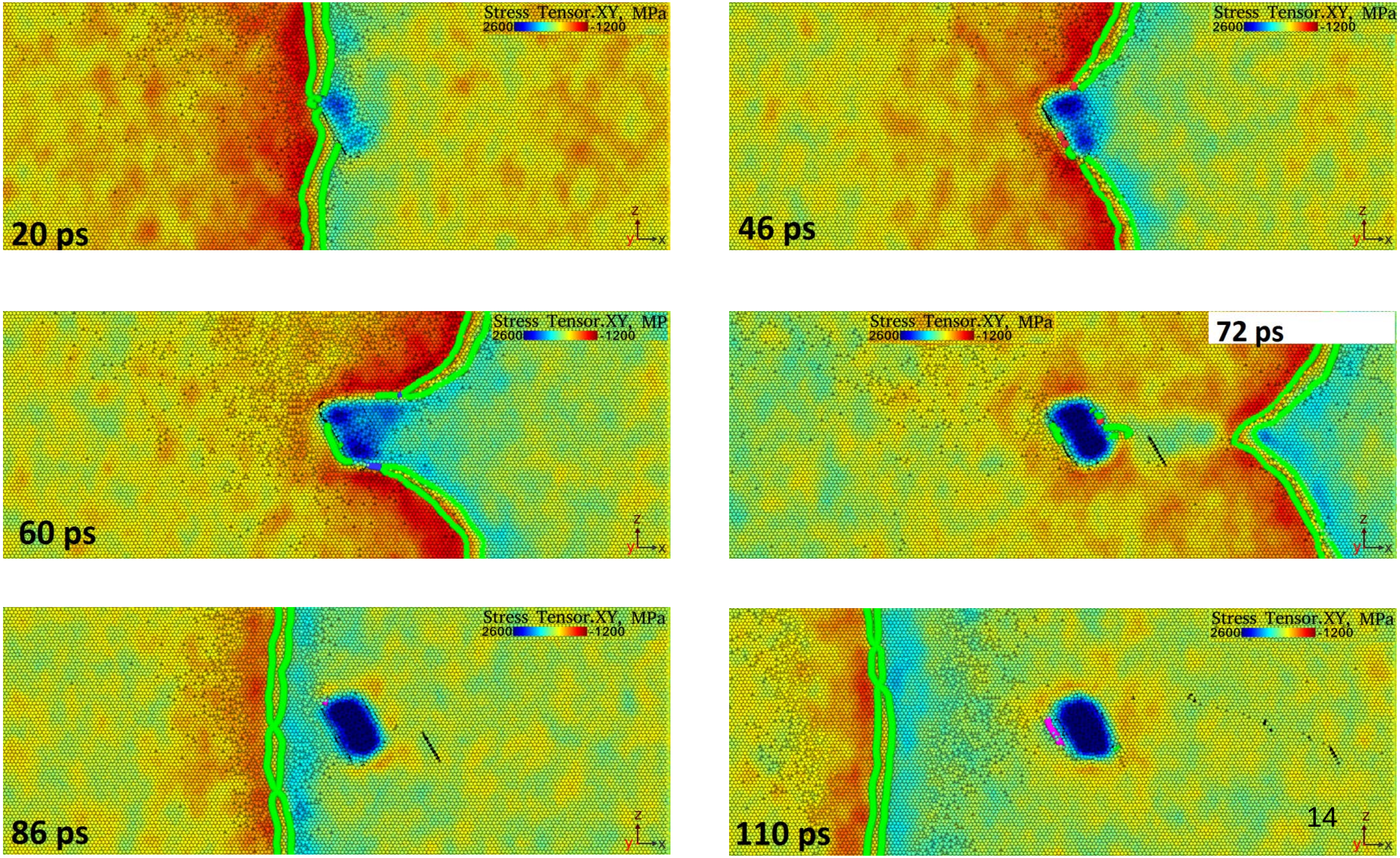
[Stukowski A., Bulatov V.V., Arsenlis A., Modelling Simul. Mater. Sci. Eng. (2012)]

[Krasnikov and Mayer, Int. J. Plast. (2019)]

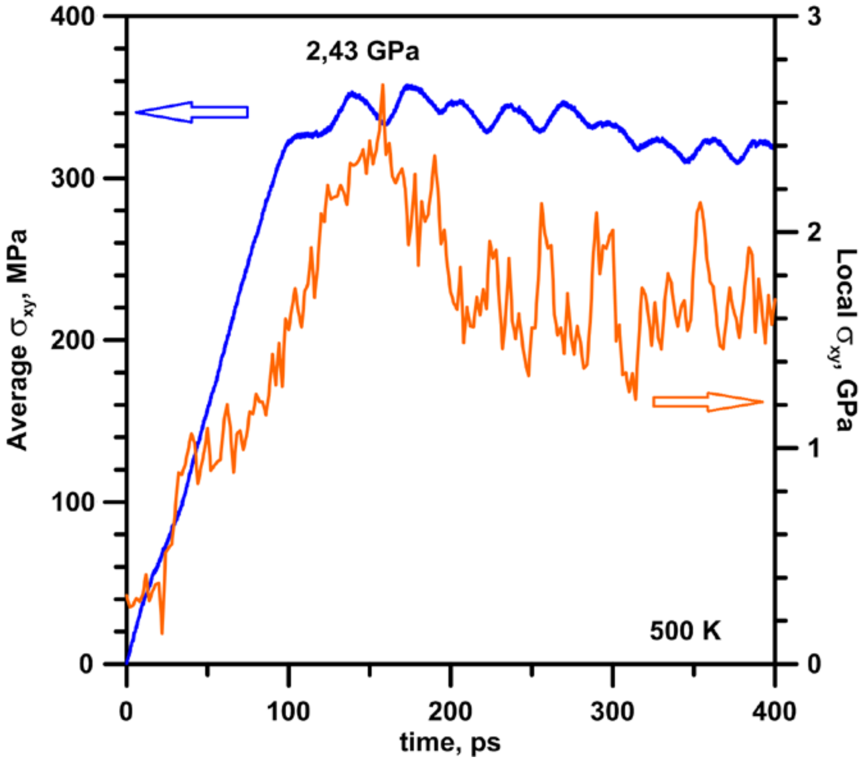
Local shear stress

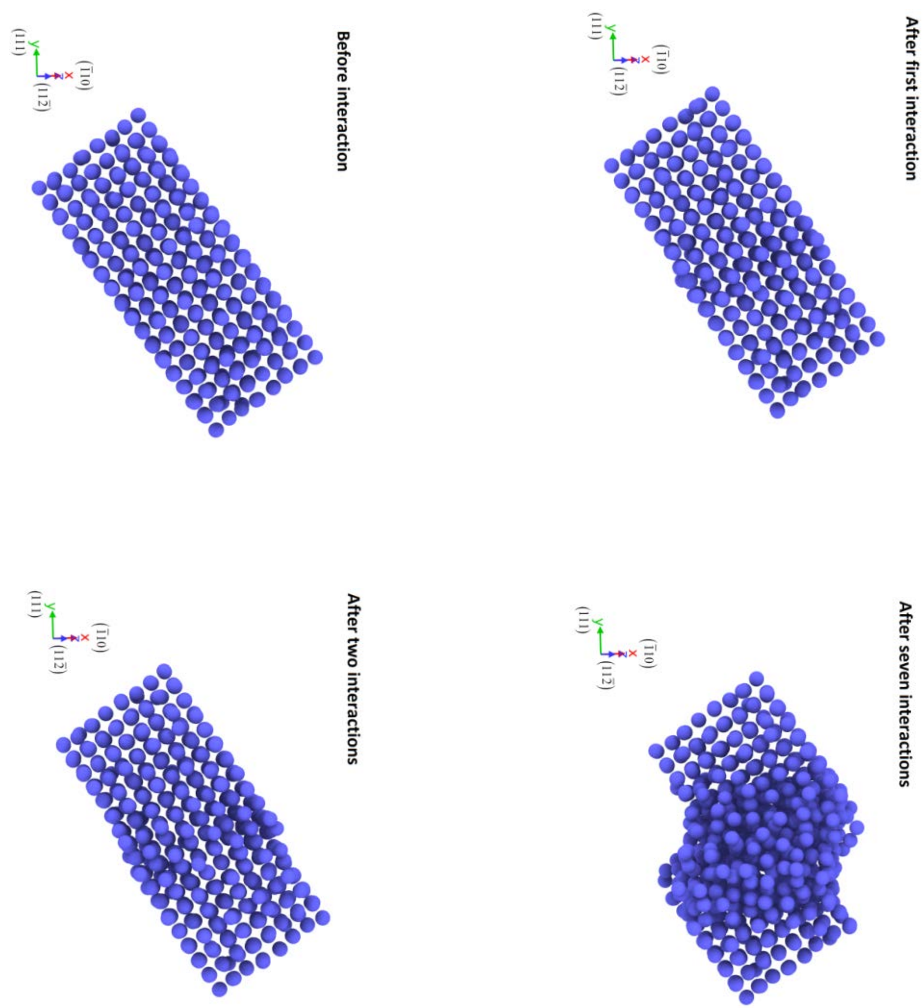
Stress_xy, MPa

2600 -1200



Local stress and inclusion shape

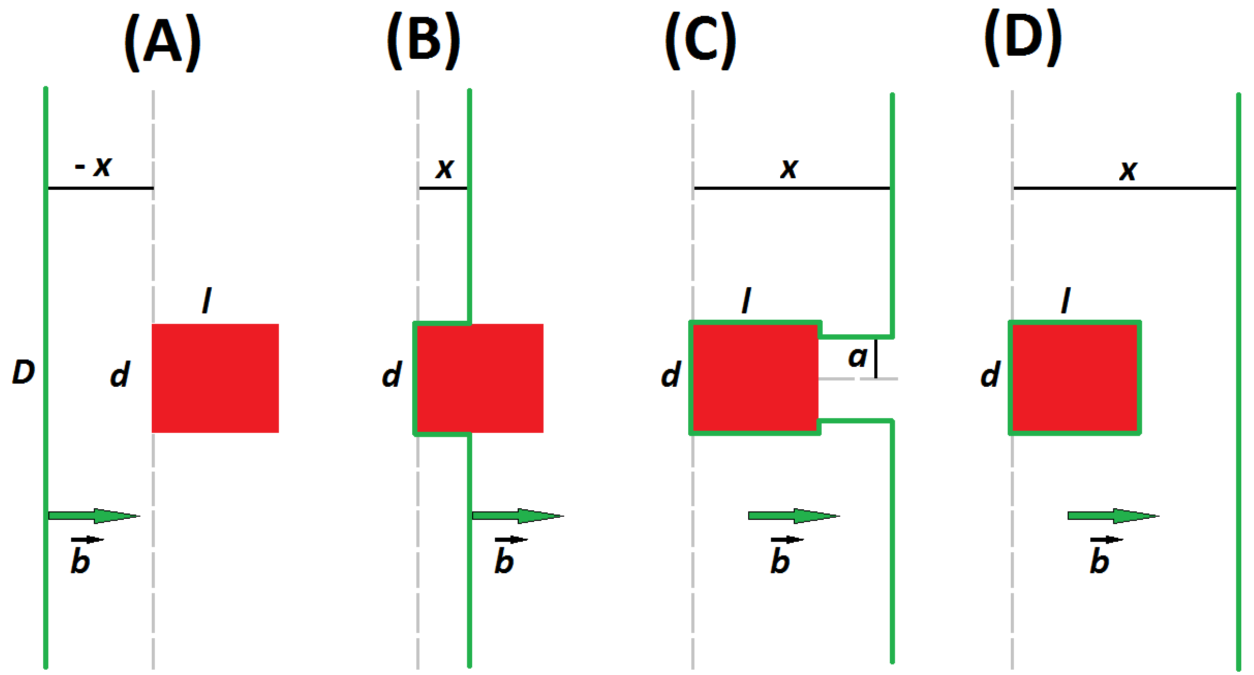




[Krasnikov and Mayer, Int. J. Plast. (2019)]

Model for dislocation motion in metal with precipitates

Interaction with precipitate: model configurations and energy of dislocation in stress field



$E = -S_D b\sigma' + L_D \varepsilon_D$ energy of the dislocation segment

S_D area swept by the dislocation segment

σ' acting shear stress

b Burgers vector

L_D length of the dislocation line segment

ε_D energy of unit length of dislocation line

[Krasnikov and Mayer, Int. J. Plast. (2019)]

$\varepsilon_D b$

Continuum model: forces and dislocation motion

Temperature (K)	$b\varepsilon_D$, eV
100	1.25
300	0.85
500	0.81
700	0.81

$$E(x,a) = -Sb\sigma' + L\varepsilon_D$$

x and a are generalized coordinates

$$f_x = -\frac{\partial E}{\partial x}, \quad f_a = -\frac{\partial E}{\partial a}$$ –generalized forces

Equations of motion:
$$m_0\ddot{x} = (f_x / L_x)\left(1-\dot{x}^2/c_t^2\right)^{3/2} - B_0\dot{x}$$

$$m_0\ddot{a} = (f_a / L_a)\left(1-\dot{a}^2/c_t^2\right)^{3/2} - B_0\dot{a}$$

L_x, L_a lengths of corresponding strait segment

m_0 rest mass of dislocation

B_0 drag coefficient

c_t transverse speed of sound

Parameter	Value
B_0	$1.45 \cdot 10^{-5}$ Pa $\times$ s
m_0	$1.1 \cdot 10^{-16}$ kg/m
σ_Y	1 MPa
a	$15b$
b	0.287 nm
G	26.2 GPa
c_t	3170 m/s

[Krasnikov and Mayer, Int. J. Plast. (2018)]

Continuum model: average and acting shear stresses

[Krasnikov and Mayer, Int. J. Plast. (2018)]

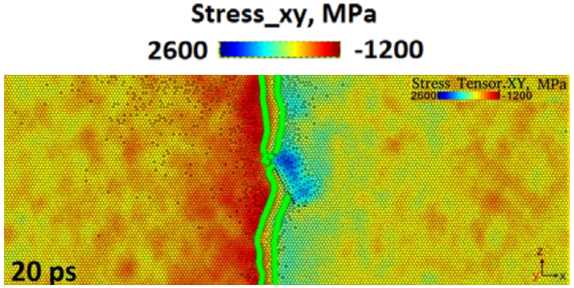
$$\langle \sigma \rangle = \frac{Gvt}{H} - \frac{Gb}{H}\frac{S}{LD}$$ average stress

H system height (in the direction perpendicular to the slip plane)

L system length (in the direction of dislocation slip)

$$\sigma = \frac{Gvt}{H} - \frac{Gb}{H}N$$ real stress in front of dislocation

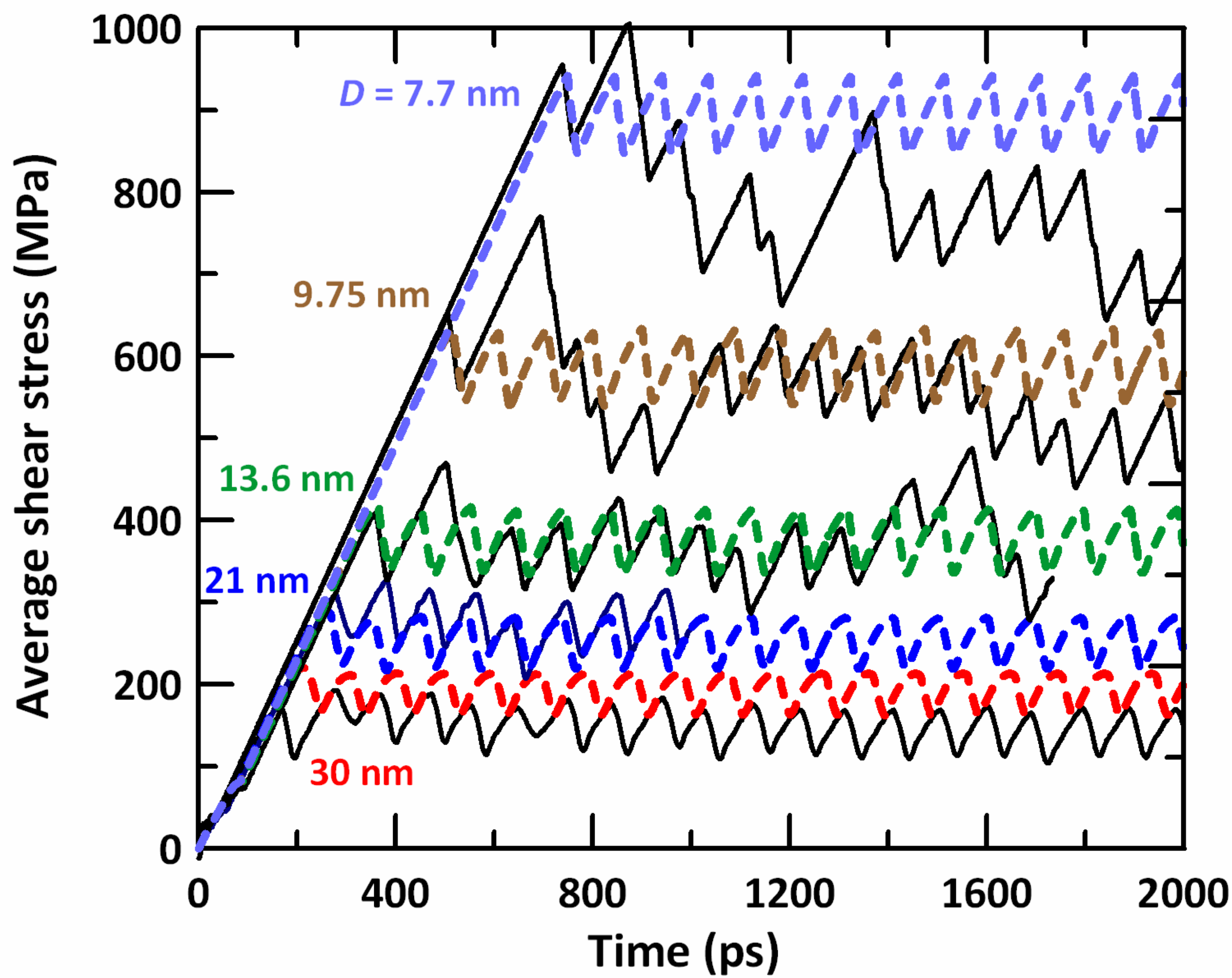
N –number of full passing through the system



a size of acting area

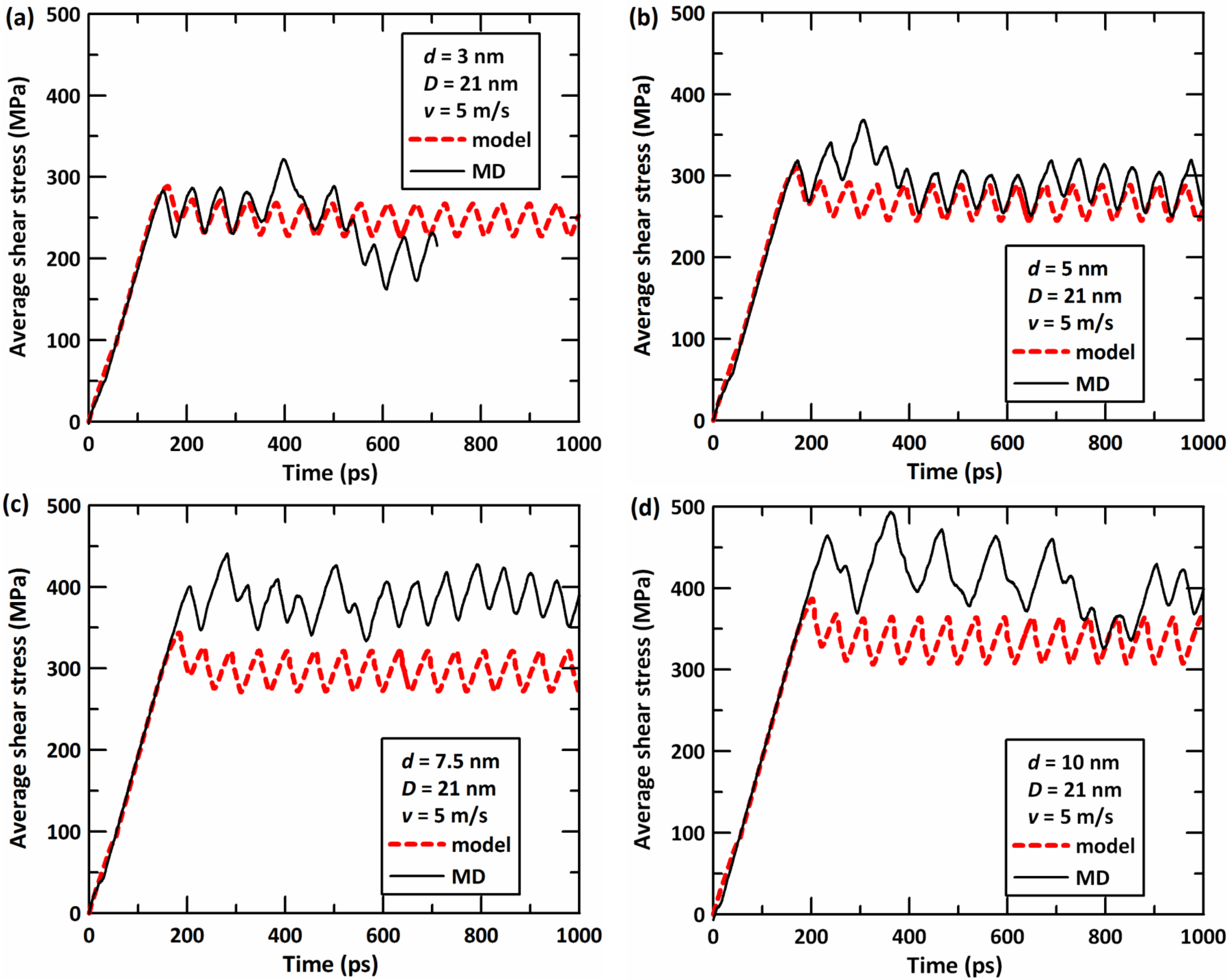
Acting stress:
$$\sigma' = \begin{cases} \sigma - \dfrac{Gb}{2H}\left(\dfrac{x}{\alpha}\right) \text{ at } (x + x_0) < \alpha, \\ \sigma - \dfrac{Gb}{2H}\left(2 - \dfrac{L-x}{\alpha}\right) \text{ at } (x + x_0) > L - \alpha, \\ \sigma - \dfrac{Gb}{2H} \text{ otherwise,} \end{cases}$$

Effect of spacing between precipitate along the dislocation line

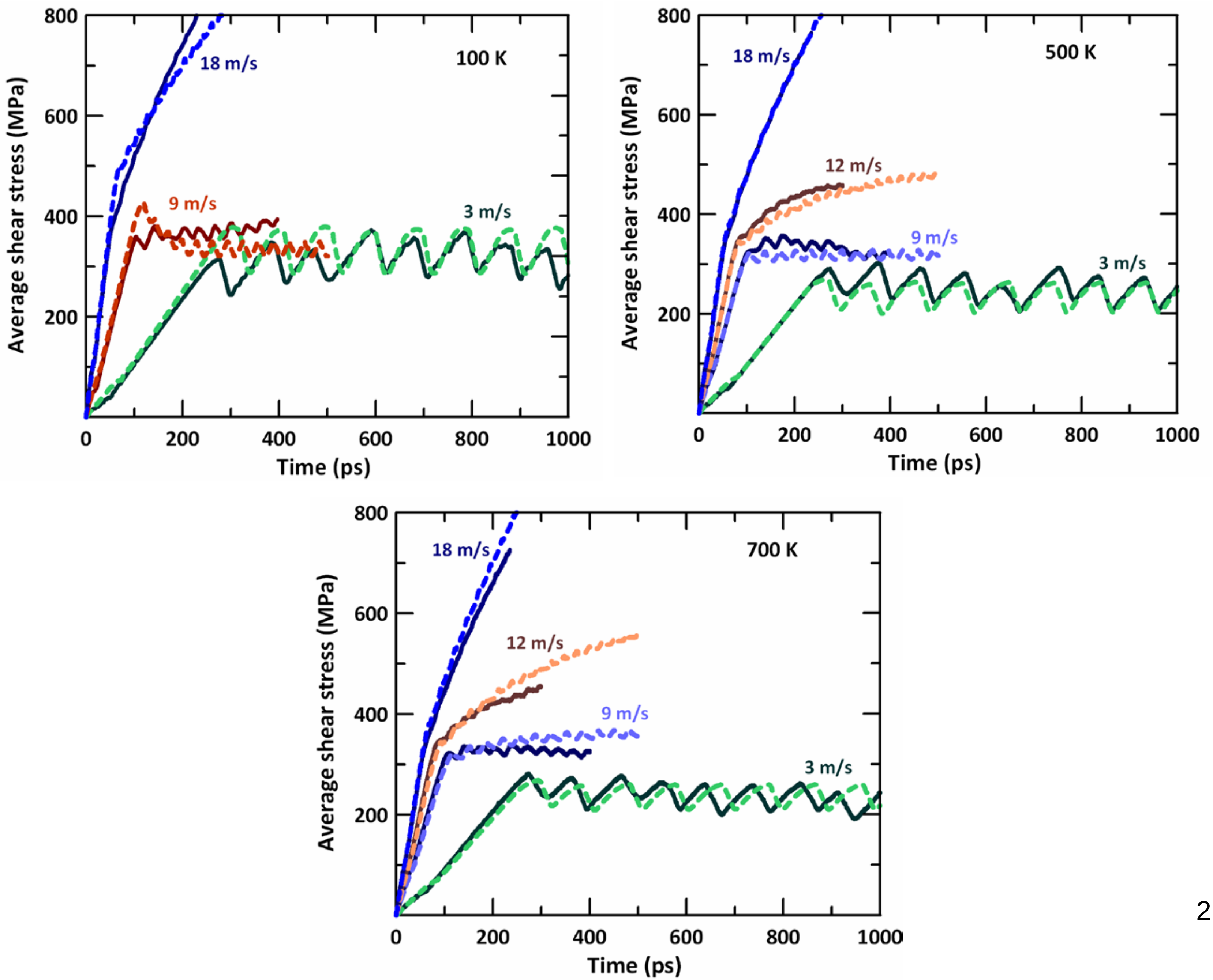


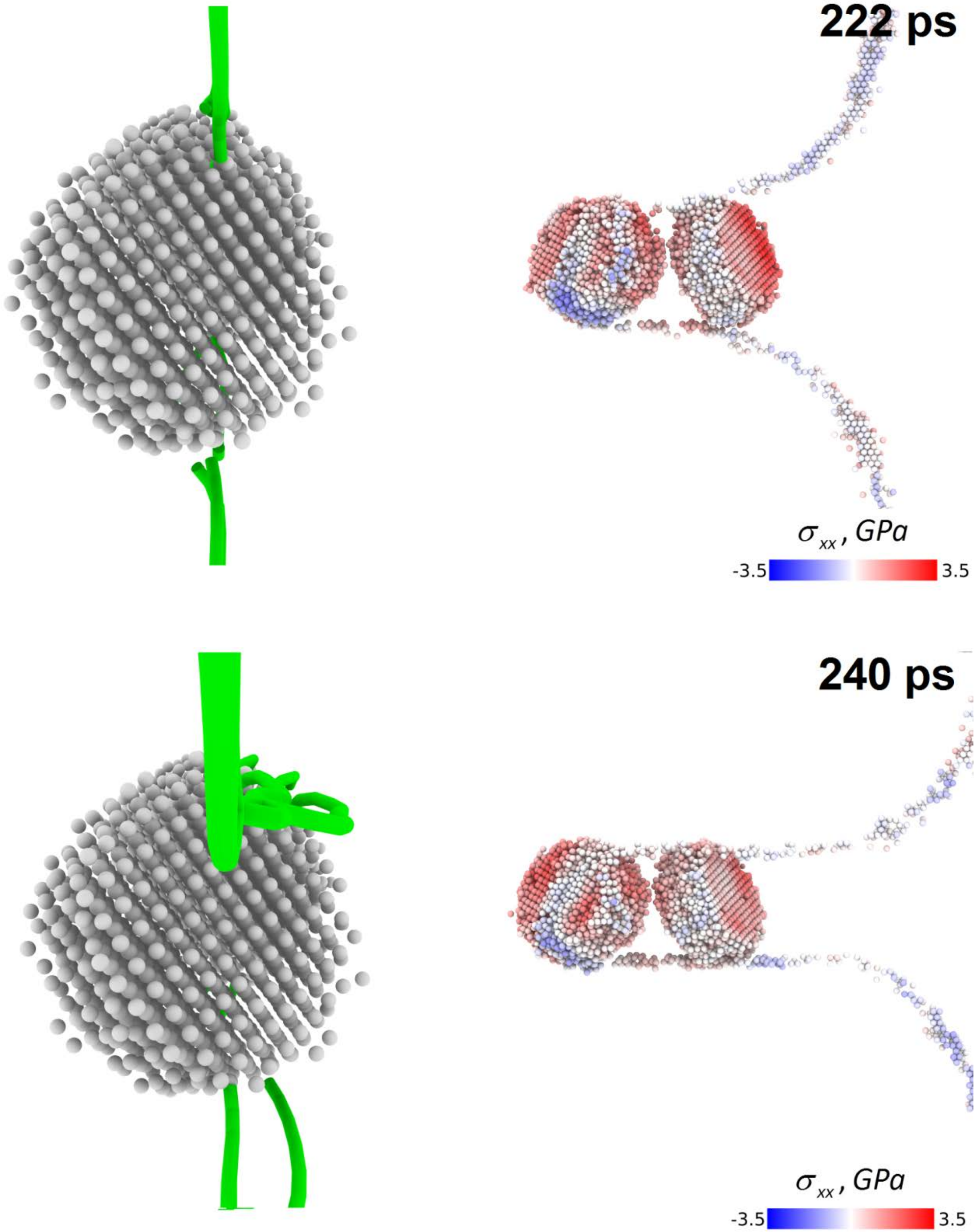
[Krasnikov and Mayer, Int. J. Plast. (2019)]

Effect of precipitate diameter



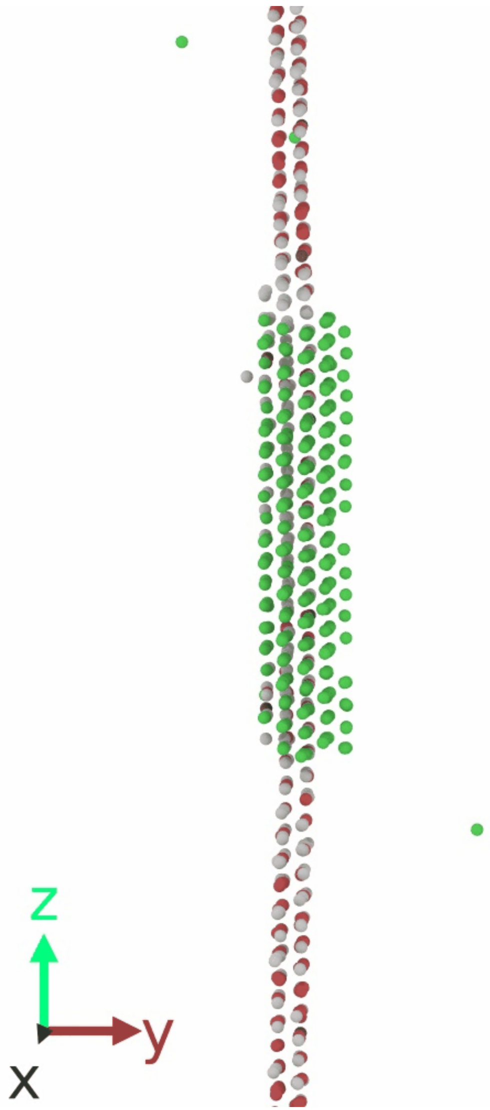
Effect of temperature

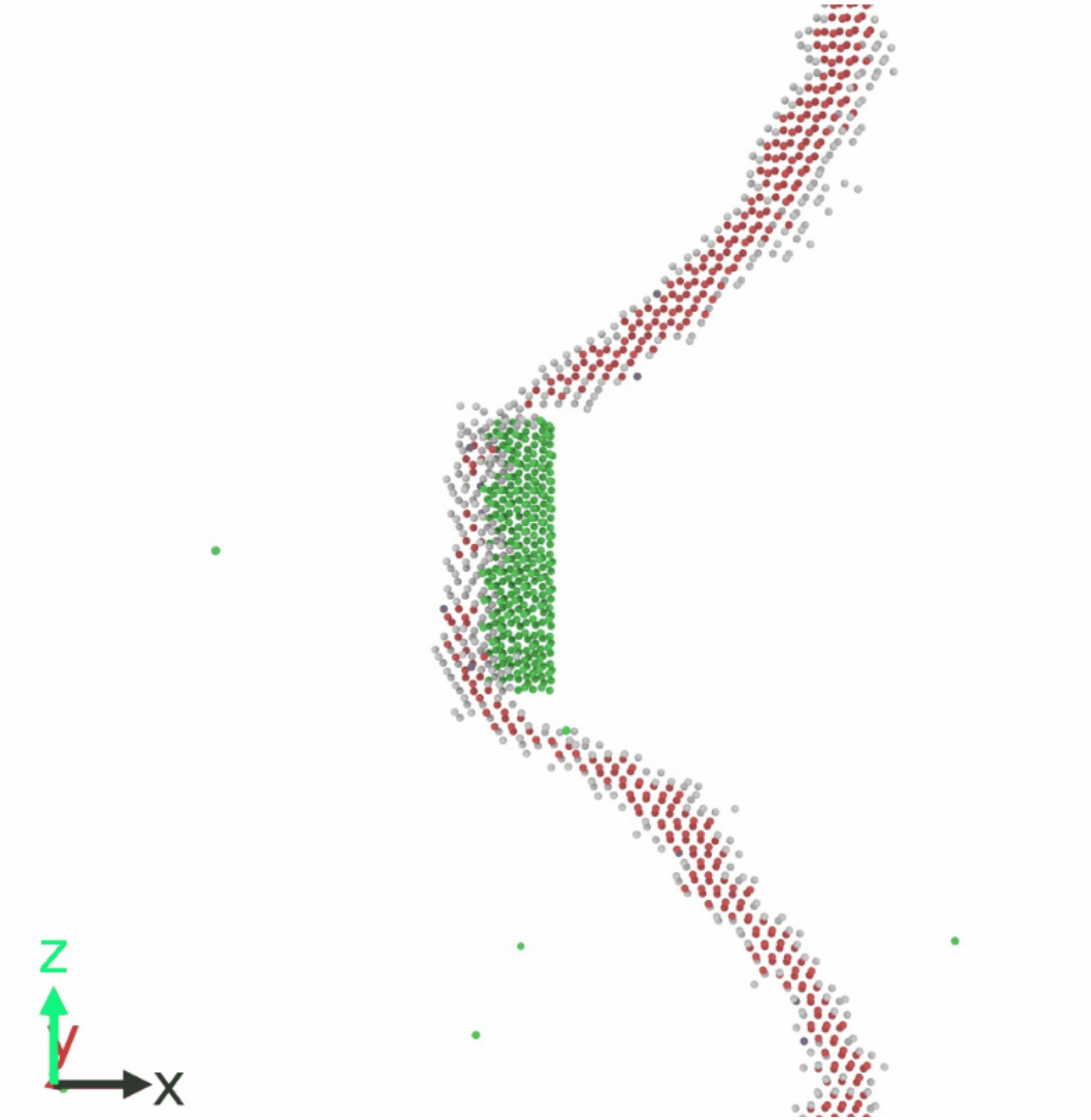




Double θ‘ precipitate:
combination of climb
And formation of loop

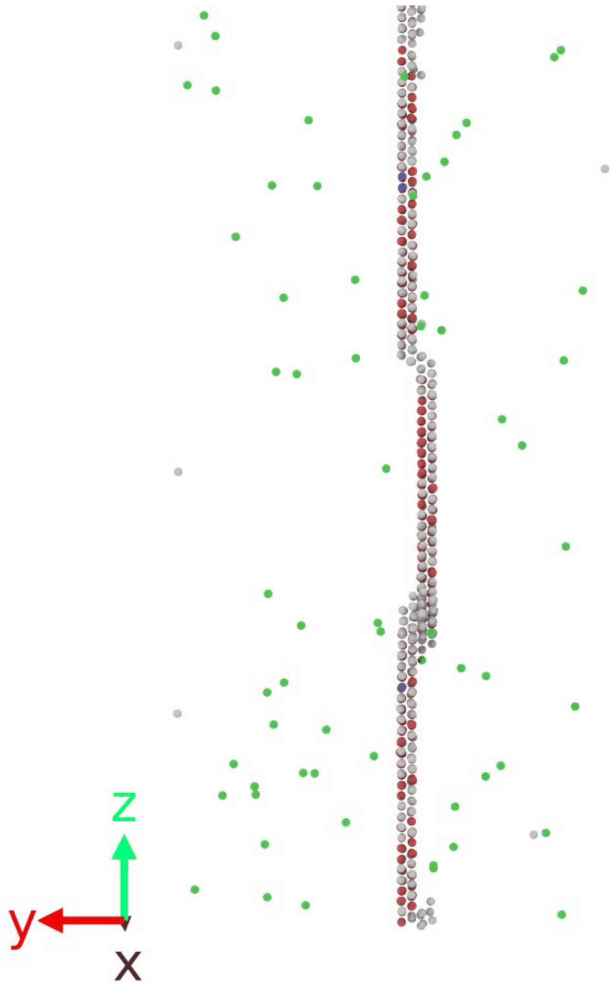
Overcoming of rigid obstacle by ejection of dislocation segment into neighboring slip plane

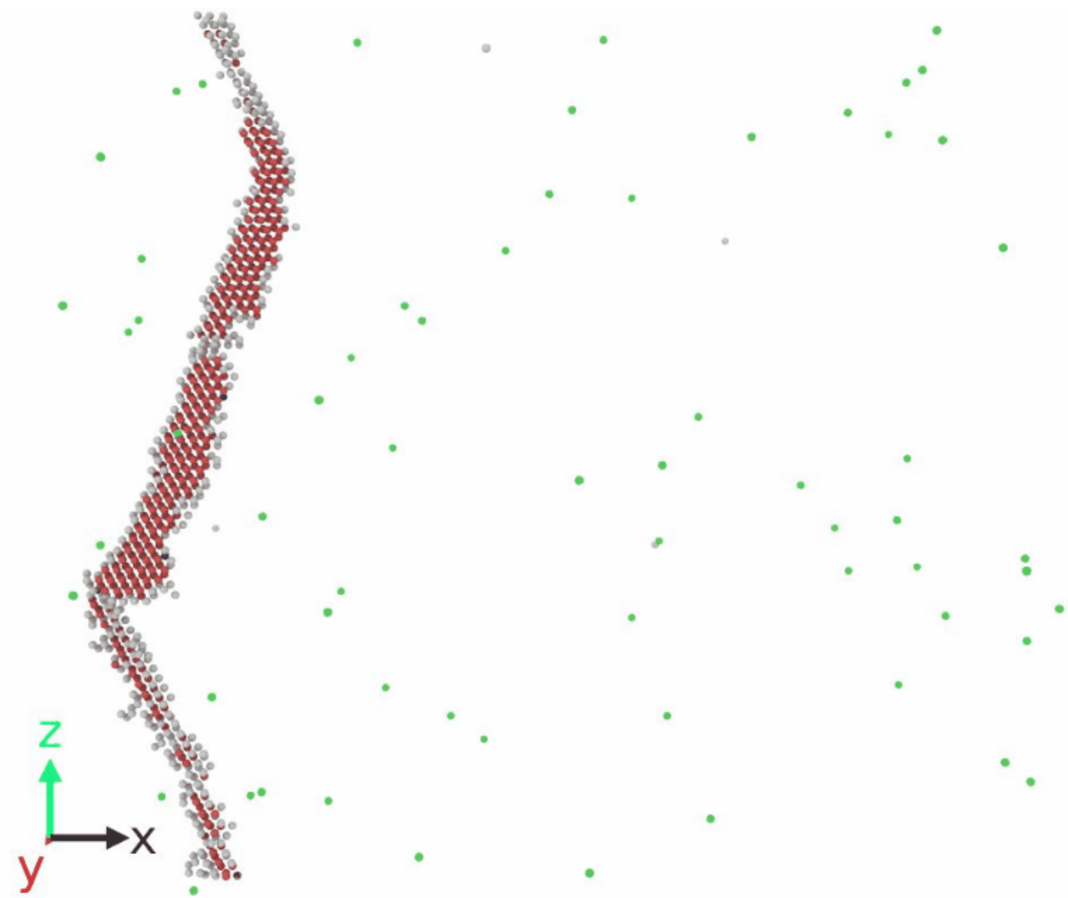




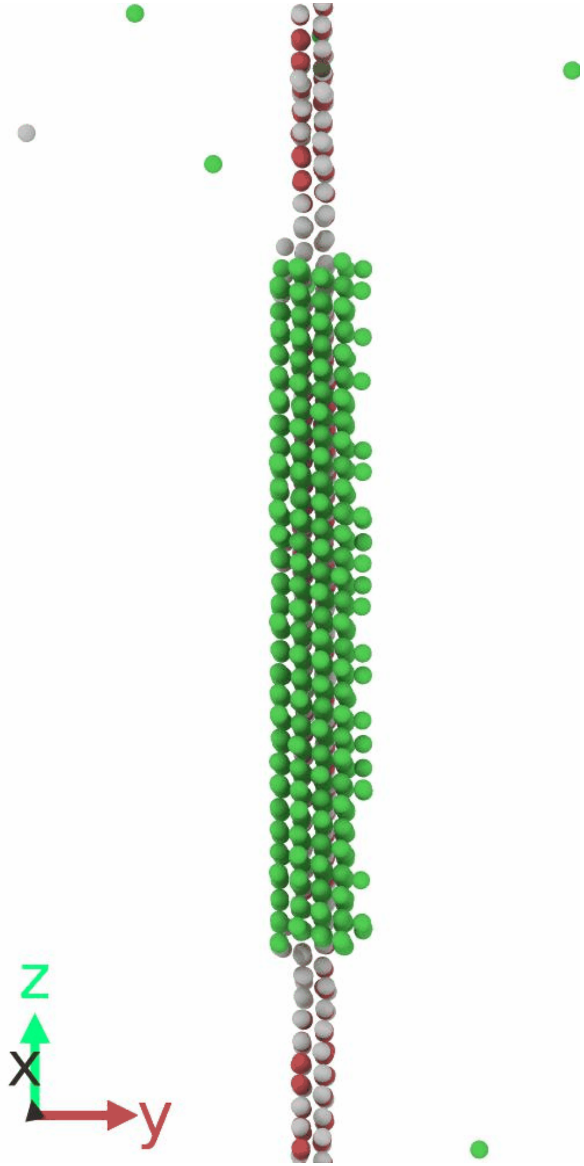
Inclusion size: 1.5 x 1 x 5 nm^3

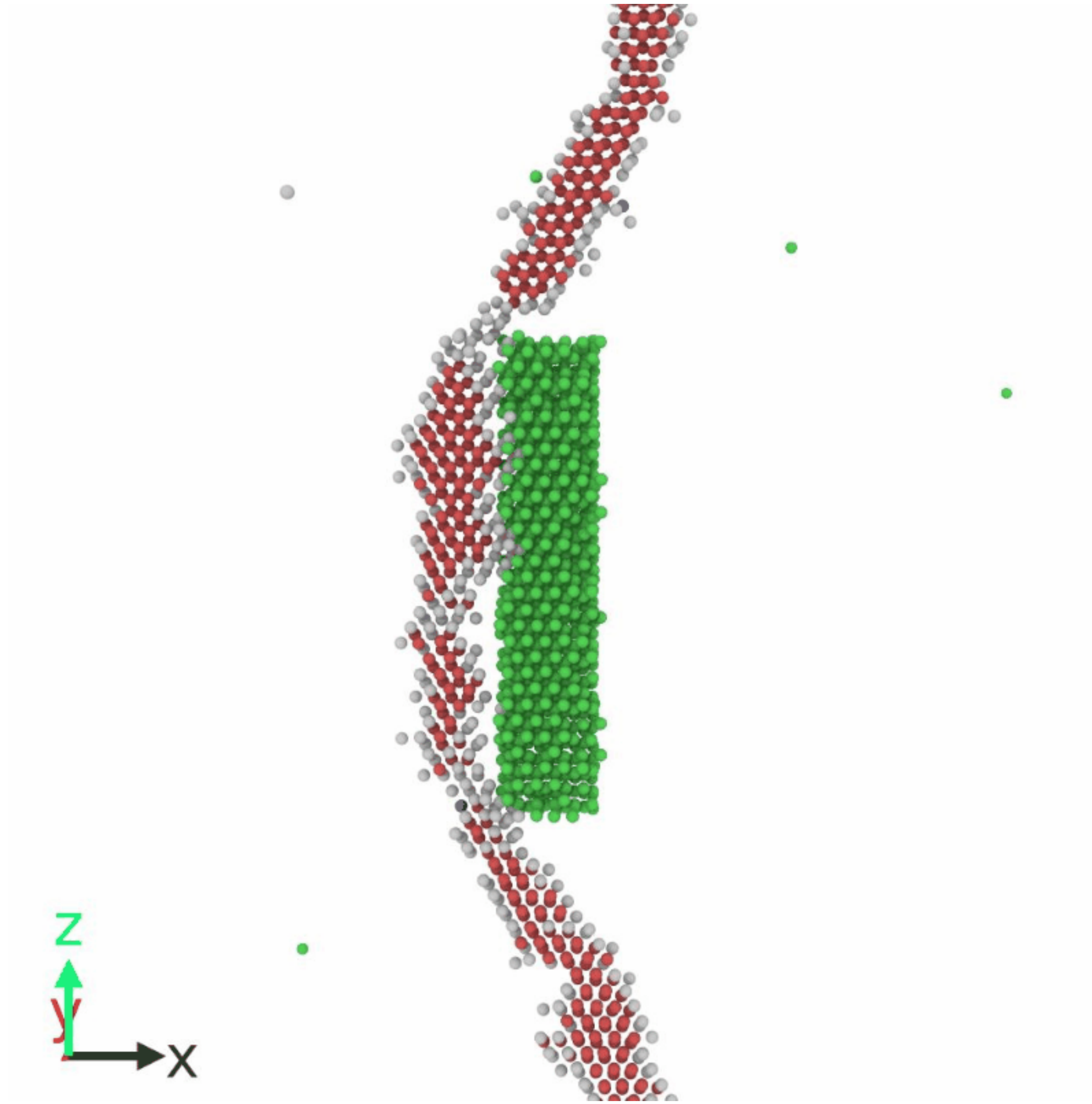
Emission of vacancies and increase in length of dislocation segment in neighboring plane





Overcoming of rigid obstacle by formation of Orowan loop

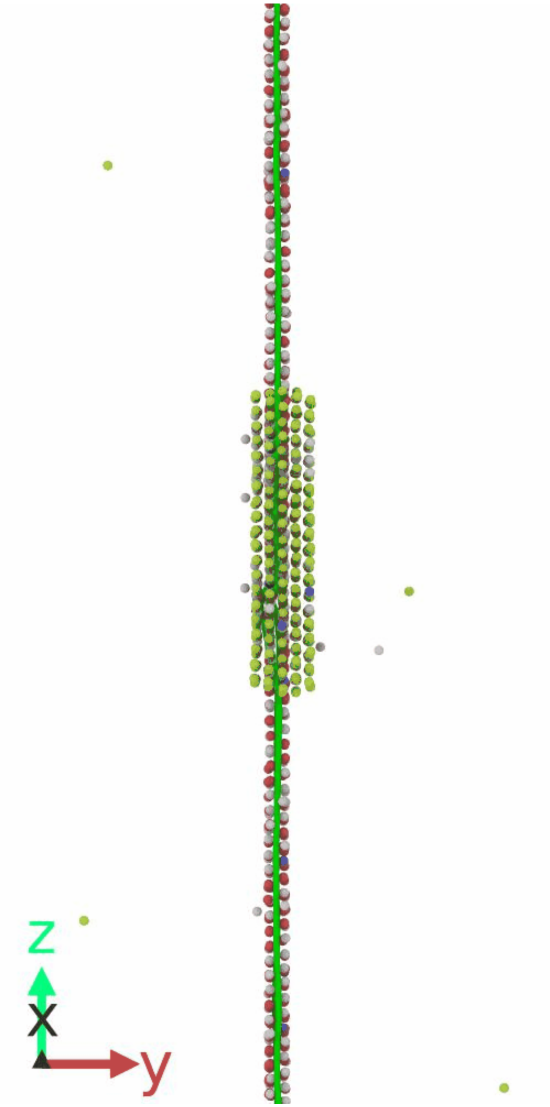


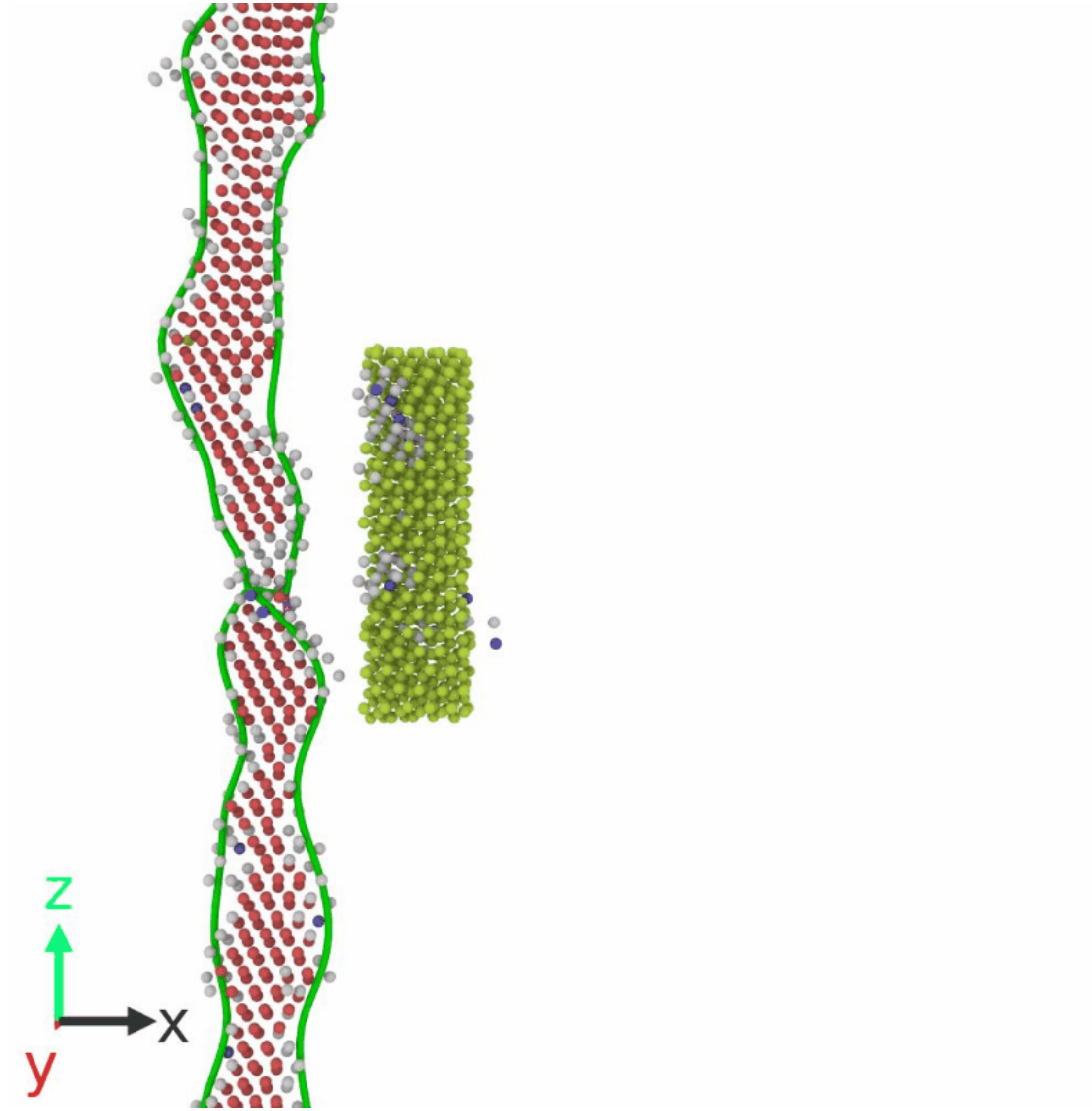


Inclusion size: 1.5 x 1 x 7.5 nm^3

Model obstacles

Overcoming of Cu obstacle by shearing





Inclusion size: 1.5 x 1 x 5 nm^3

Kinetics of dislocations

Mobile dislocations $\frac{d\rho_D^\beta}{dt} = Q_N^\beta + Q_D^\beta - Q_I^\beta - Q_{Da}^\beta$

Immobilized dislocations $\frac{d\rho_I^\beta}{dt} = Q_I^\beta - Q_{Ia}^\beta$

$$Q_N^\beta = \frac{c_t}{b^3}\exp\left(-\frac{\pi\varepsilon_D^2 / \left(\mathbf{b}^\beta \cdot \mathbf{S} \cdot \mathbf{n}^\beta\right)}{kT}\right)$$

Nucleation

$$\boxed{Q_D^\beta = \frac{\eta}{\varepsilon_D}\left(\mathbf{b}^\beta \cdot \mathbf{S} \cdot \mathbf{n}^\beta\right) V_D^\beta \rho_D^\beta}$$

Multiplication

$$Q_I^\beta = V_I\left(\rho_D^\beta - \rho_0\right)\sqrt{\rho_I^\beta}$$

Immobilization

$$Q_{Da}^\beta = k_a b\left|V_D^\beta\right|\rho_D^\beta\left(\rho_D^\beta + \rho_I^\beta / 4\right) \qquad Q_{Ia}^\beta = k_a b\left|V_D^\beta\right|\rho_D^\beta\rho_I^\beta / 4$$

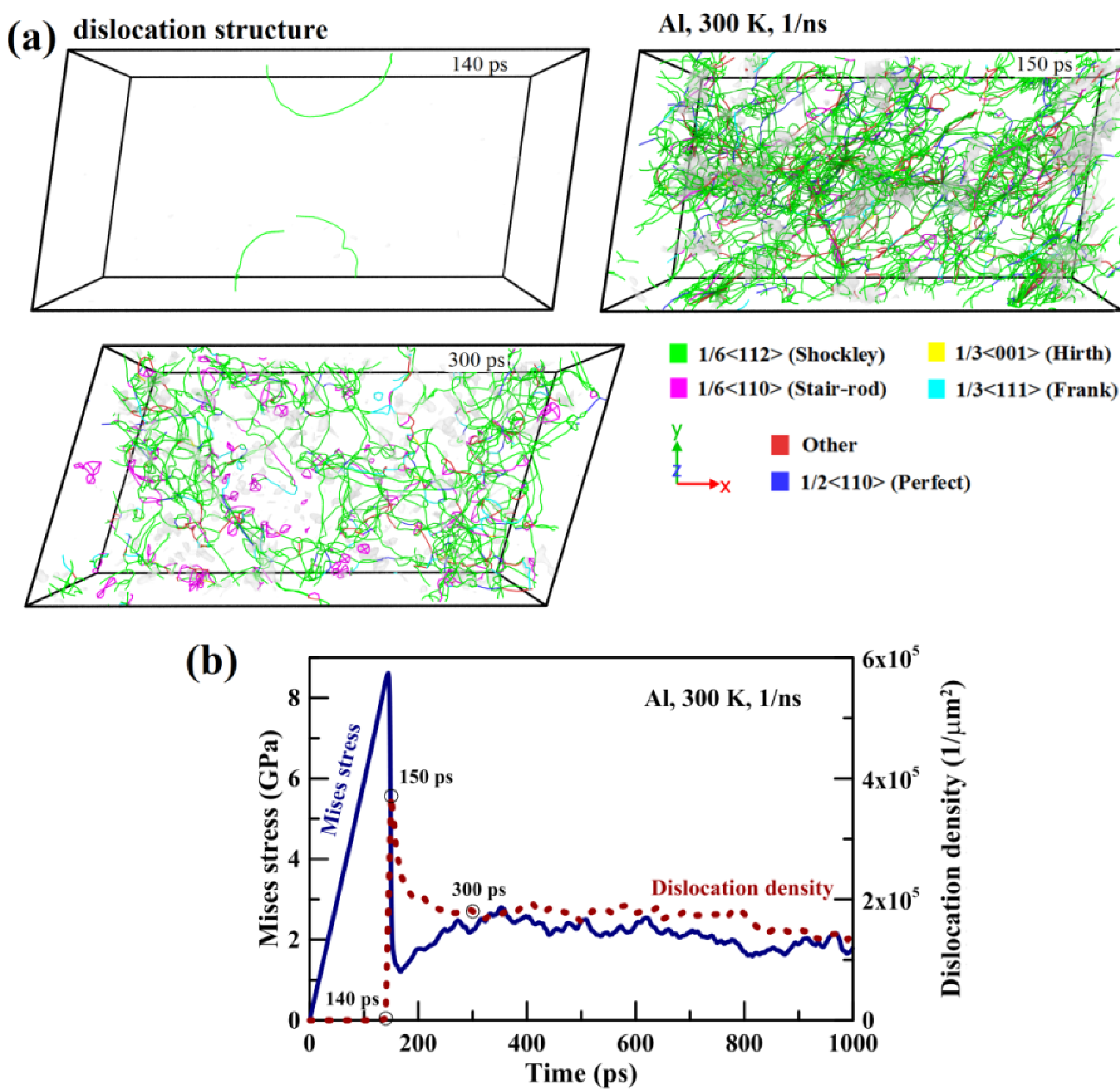
Annihilation

$\eta \approx 0.1$ - the part of dissipated energy spending on formation of defects

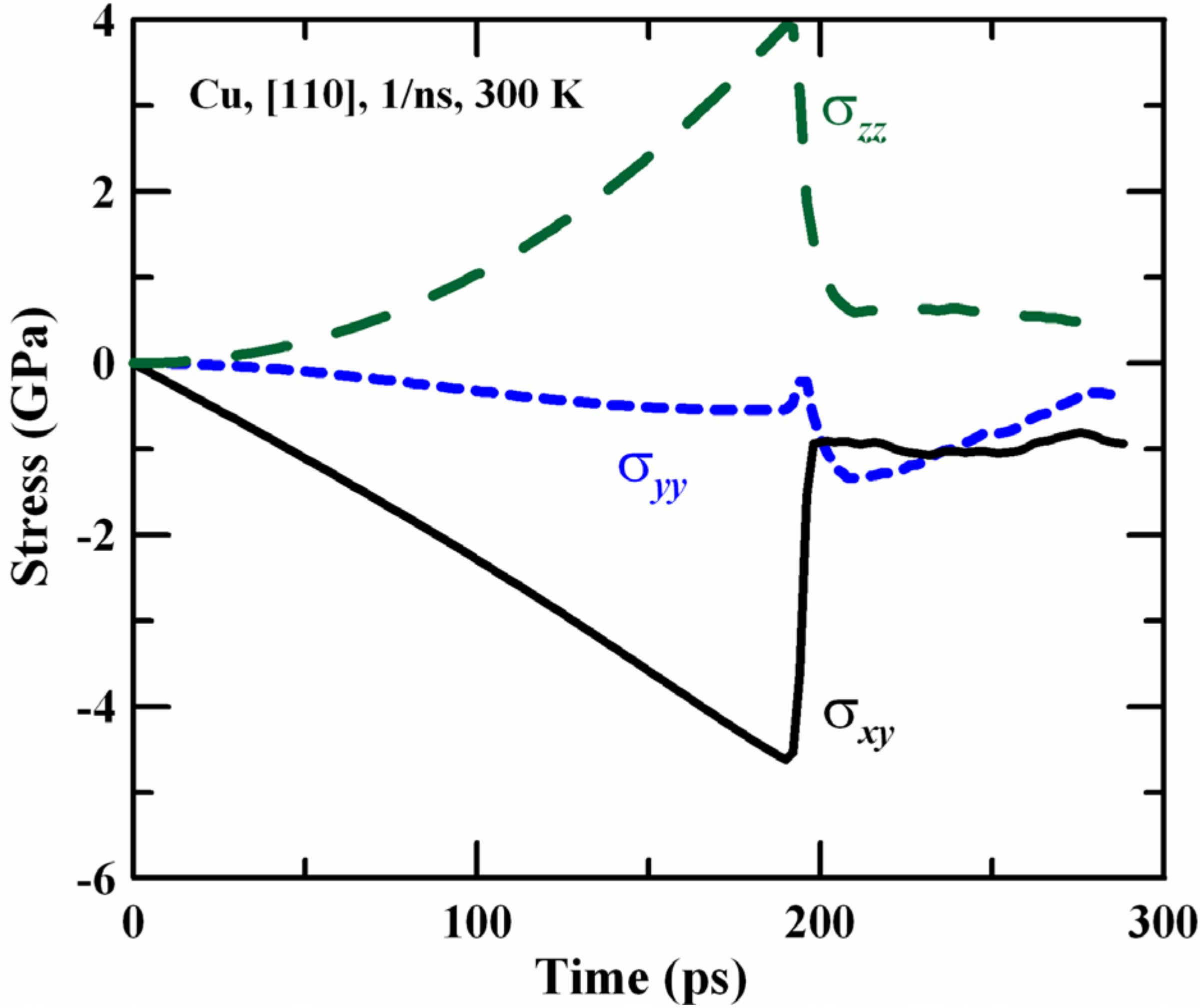
$Y = Y_0 + AGb\sqrt{\rho_I}$ - Taylor hardening law

MD simulations of pure shear

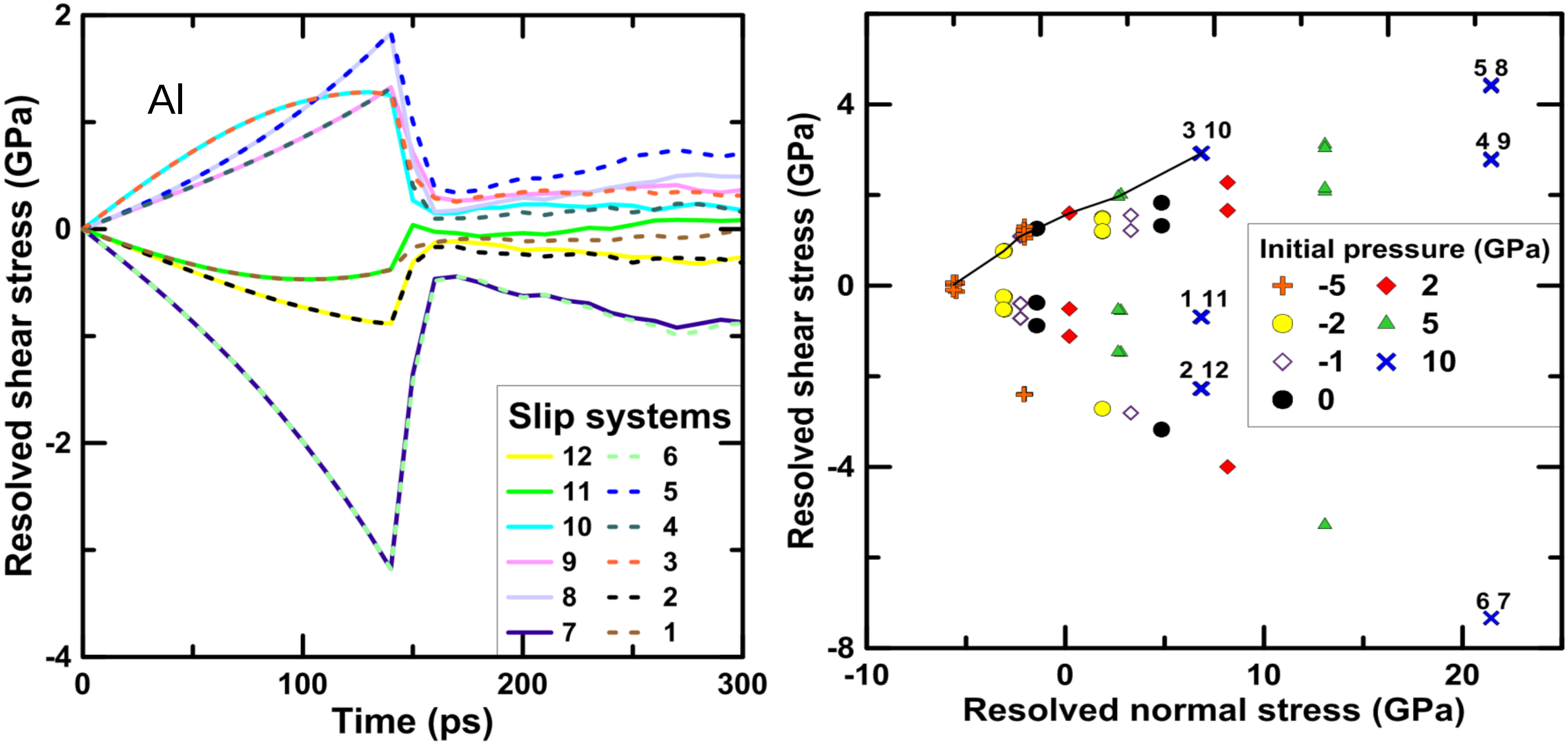
Mayer, Krasnikov and Pogorelko, Proc. ICTAEM1 (2019)



Complexity: non-linear stresses



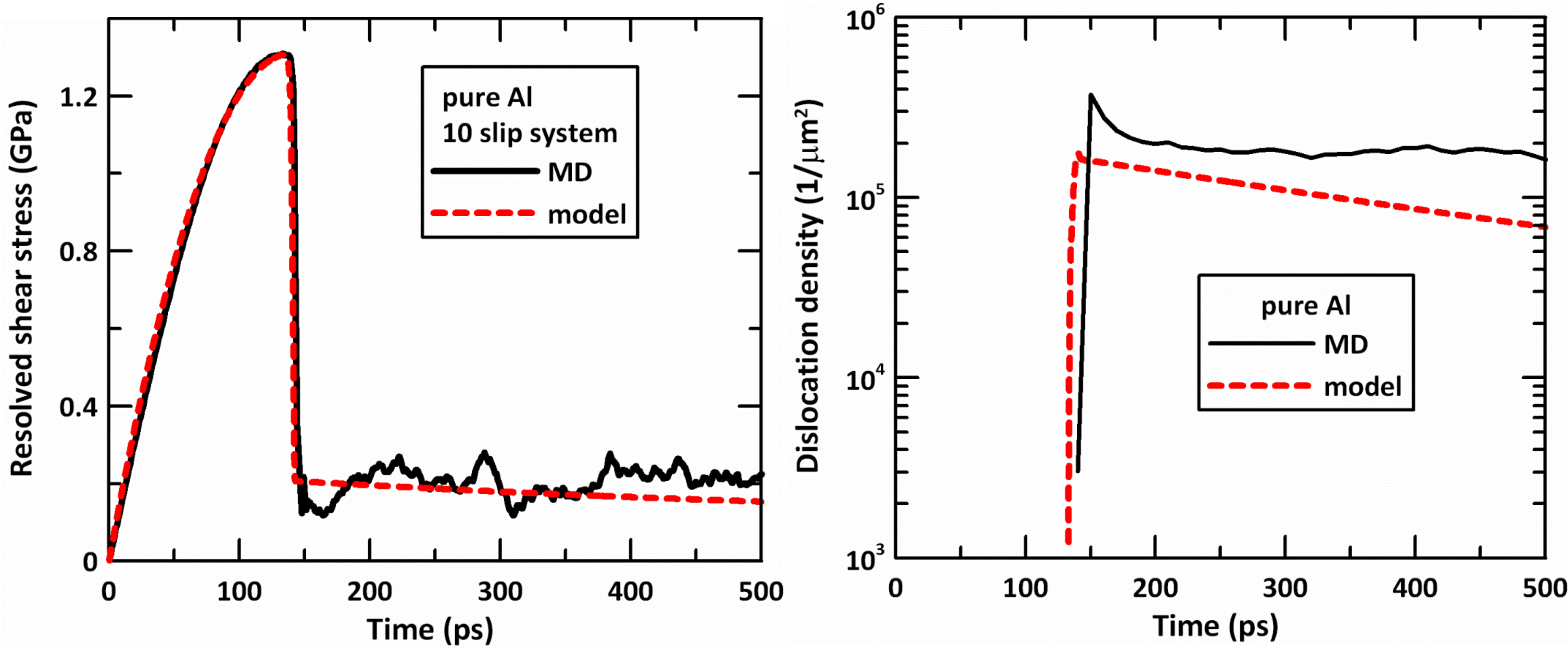
Resolved shear stress



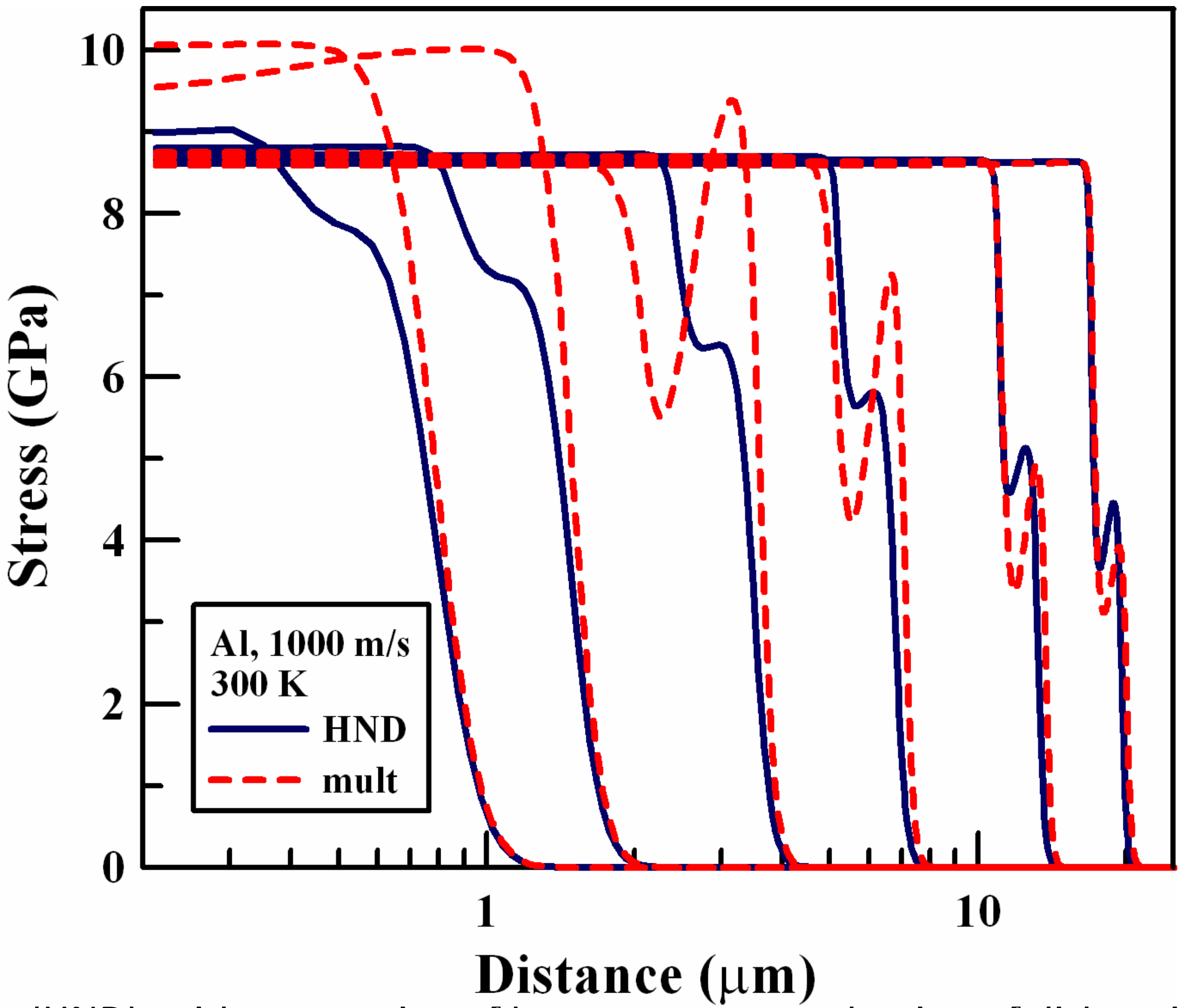
$$RSS = \left(\mathbf{b}/b\right) \cdot \mathbf{S} \cdot \mathbf{n}$$

$$RNS = \mathbf{n} \cdot \mathbf{S} \cdot \mathbf{n}$$

Comparison of MD and model

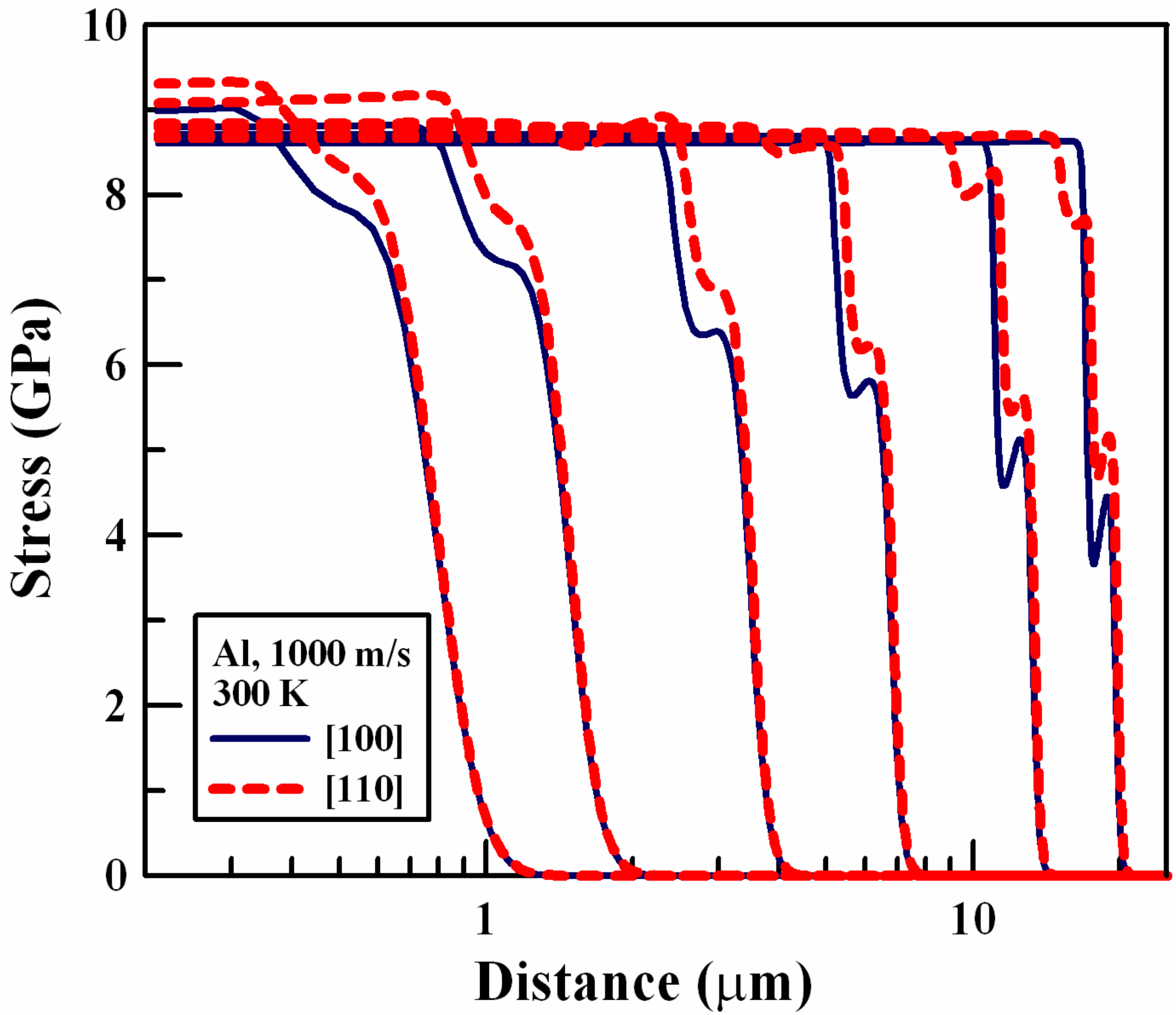


Shock waves in thin samples: influence of homogeneous nucleation



solid lines (HND)–with accounting of homogeneous nucleation of dislocations
dash lines (mult)–without HND, only multiplication of dislocations
Al single crystal, direction of the shock wave loading is [100]

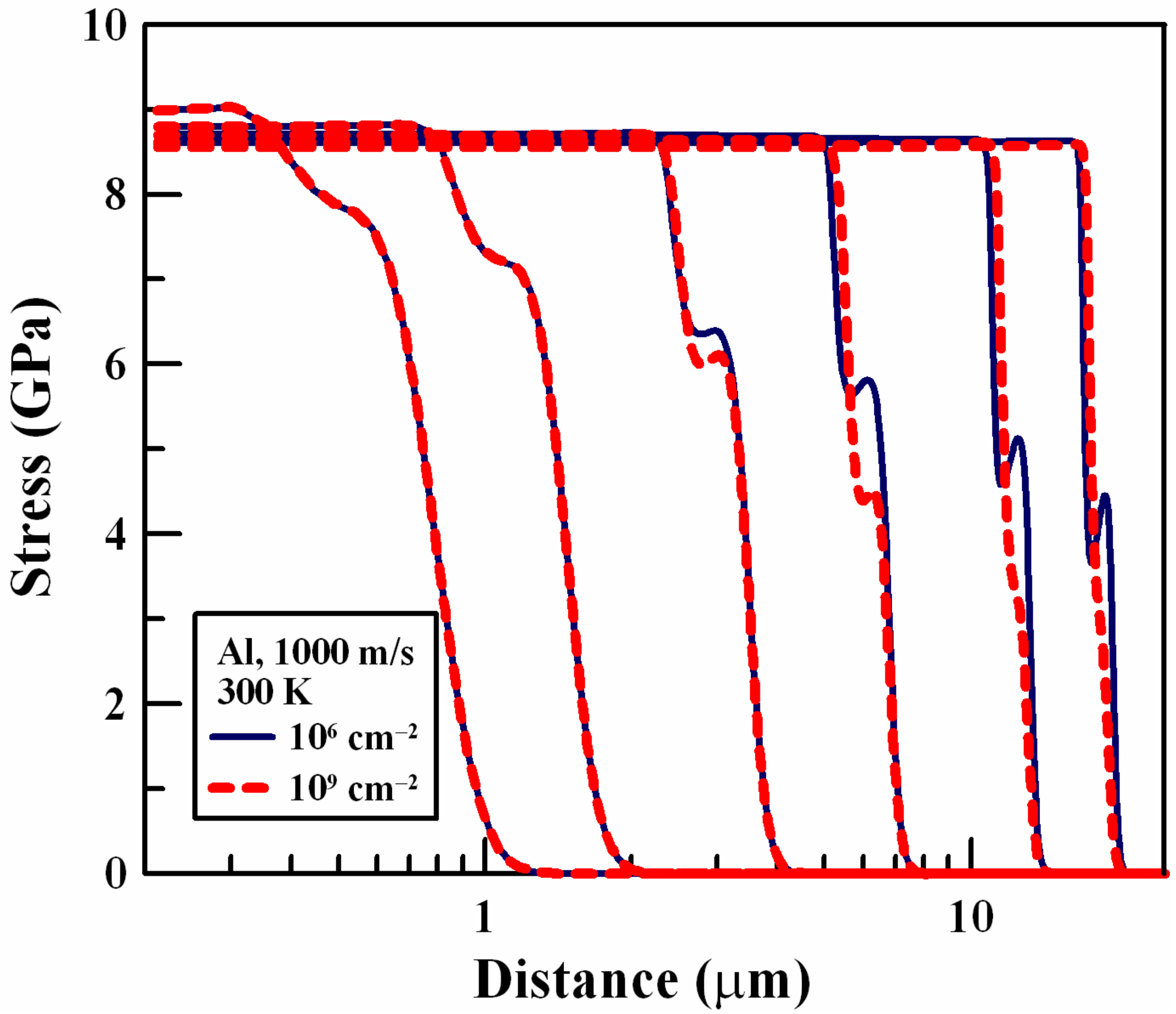
Shock waves in thin samples: influence of loading direction



Two shock waves–activation of additional slip systems at saturation of dislocation density in primary slip systems

Similar result for BCC Ta [Djordjevic, Vignjevic, Kiely, Case, De Vuyst, Campbell and Hughes, Int. J. Plast. (2018)]

Shock waves in thin samples: influence of initial dislocation density



Conclusions

- Continuum model with accounting of dislocations is used for description of material behavior in dynamic deformation conditions
- Equations of dislocation motion and generation are constructed basin on MD simulation analysis, and the model parameters are determined from MD
- Motion of dislocation in pure metal is effected by local stress, which can considerably differ from the average one
- Overcoming of obstacles (precipitates) goes by looping for largeer obstacles or ejection of segment for smaller one. Shearing of precipitate is a secondary process.
- Nucleation of dislocation in perfect crystal occurs near the lattice instability point and considerably effected by nonlinear elastic behavior of crystal at large strains

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