Multiscale modeling of dynamical plasticity of Al-Cu alloy

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Mechanisms of alloy strengthening

- inherent strength of metal matrix, usually includes the Peierls barrier;
- hardening by forest dislocations;
- grain boundaries;
- precipitates of second phases;
- pile-up of dislocation on precipitates.

(Fribourg et al., 2011; Anjabin et al., 2013; de Vaucorbeil et al., 2013; Bardel et al., 2015; Anjabin, 2019; Li et al., 2019; Bellon et al., 2020; Li et al., 2020; Chen et al., 2020; Ji et al., 2020; Zhou et al., 2020a; Bahl et al., 2021)

Sequence of strengthening phases in Al-Cu

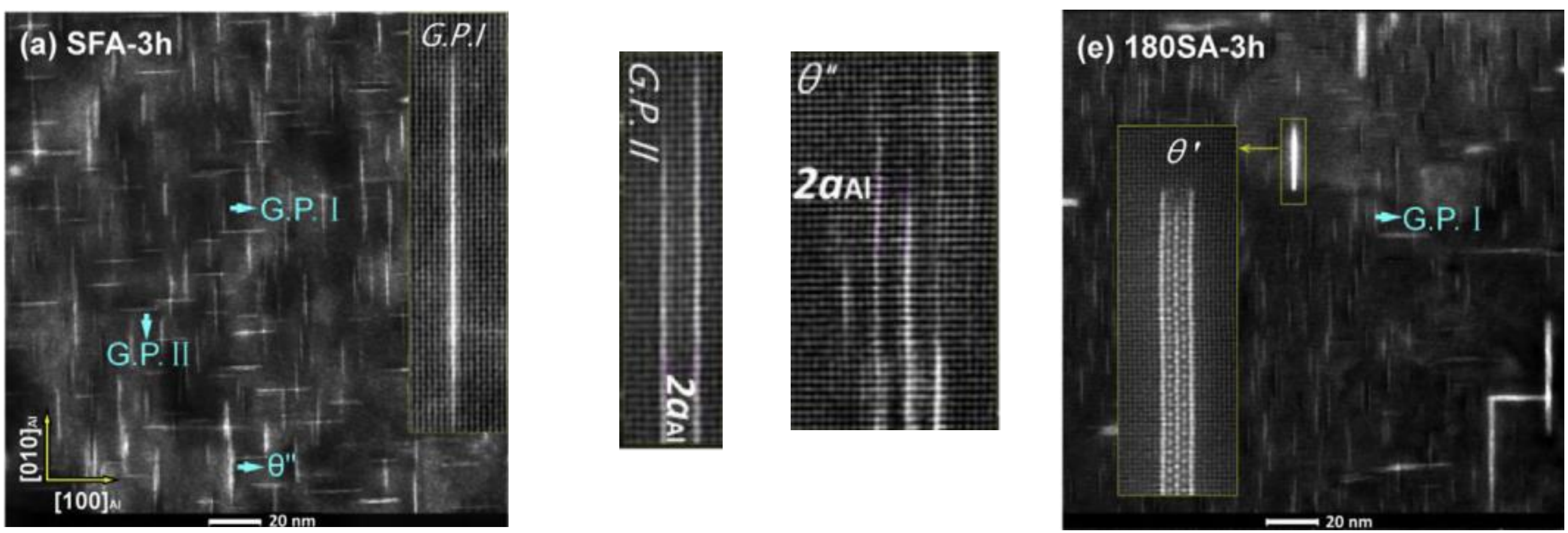
Strengthening phases in Al-Cu system released during ageing:

Solid solution → GP zones$_{1,2}$→ θ’’ → θ’ → θ

Depending on aging conditions sizes of precipitates vary in range from units to hundreds of nanometers.

GP zones, θ’’ and θ’ are parallel to (100) planes of aluminum.

Relative orientation of θ and Al lattice have several realization.



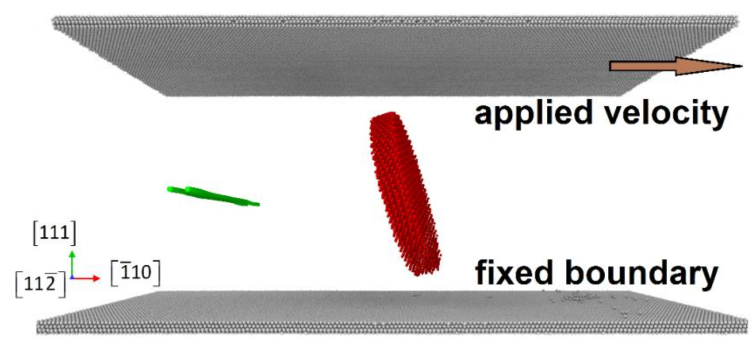
STEM images of the Al-Cu alloy samples from (Ma et al., 2018. Int. J. Plast. 110, 183–201)

Multiscale approach

- Molecular dynamics simulations of dislocation-precipitate interactions;
- Model of dislocation-precipitate interactions;
- Mesoscale modeling (2D discrete dislocation dynamics).

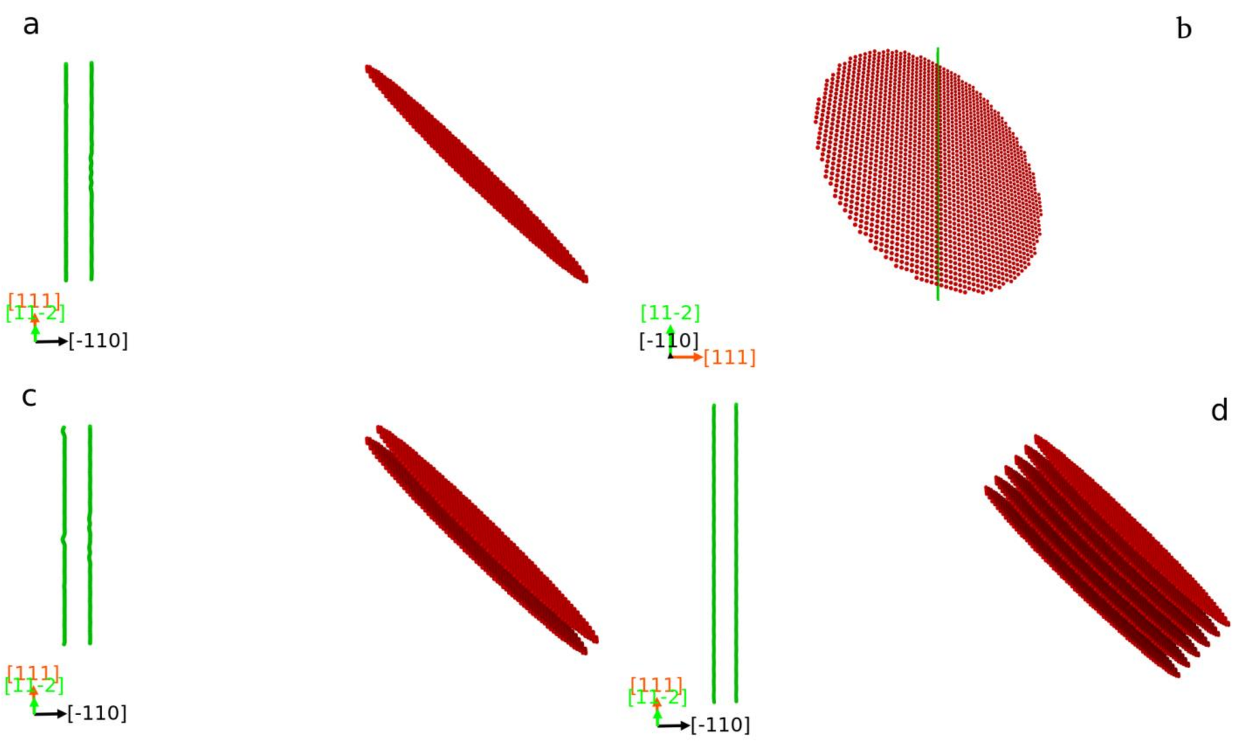
MD simulations of dislocation-precipitate interactions

- LAMMPS package (Plimpton et al.) is used;
- Angle Dependent Potential for Al-Cu (Apostol and Mishin, 2011);
- Analysis and visualization with Ovito package (Stukowsky et al.)
- Movement of dislocation is studied with scheme proposed in (Daw et al., 1992) for the slip system $[\bar{1}\,1\,0](1\,1\,1)$;
- Initially perfect edge dislocation is introduced into system, and divides into two partials in accordance with reaction $1/2\,[\bar{1}\,1\,0] \rightarrow 1/6\,[\bar{2}\,1\,\bar{1}] + 1/6\,[\bar{1}\,2\,1]$;
- Deformation is applied by shifting upper boundary of MD system;
- Temperature is controlled by thermostat.



GP zones and θ’’ phases

GP zones and θ” phase are disk of one, two or more parallel layers of copper atoms separated by three layers of aluminum atoms

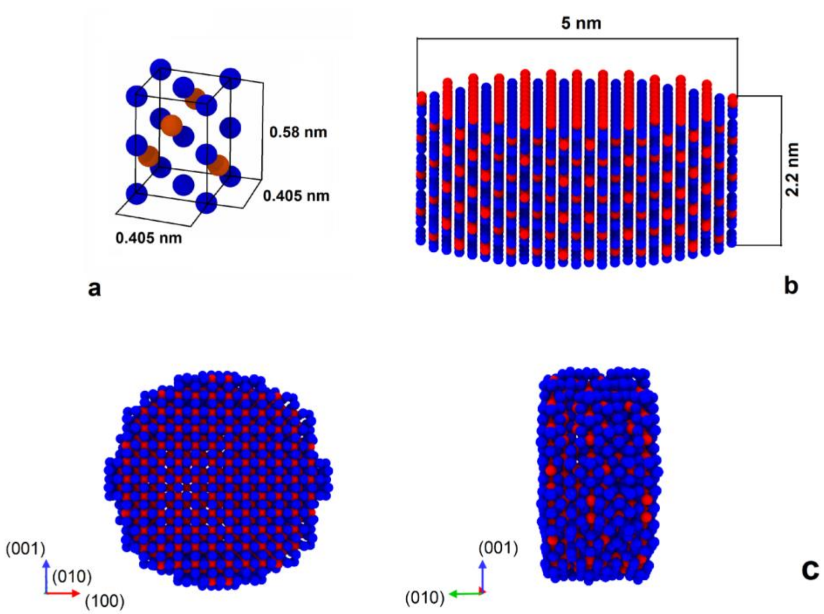


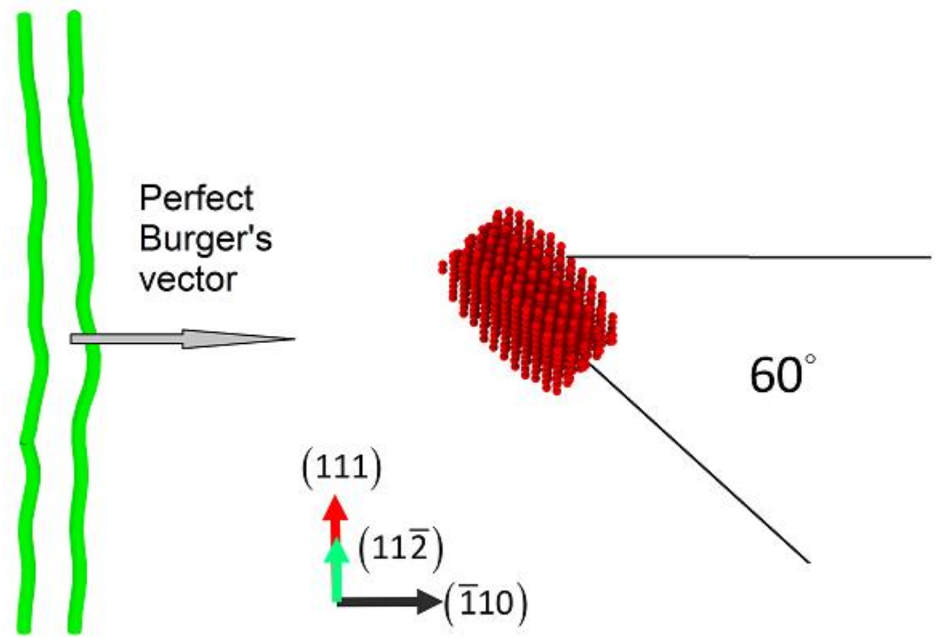
Yanilkin, A.V., Krasnikov, V.S., Kuksin, A.Yu., Mayer, A.E., 2014. Int. J. Plast. 55, 94-107;
Krasnikov, V.S., Mayer, A.E., Pogorelko, V.V., Latypov, F.T., Ebel, A.A., 2020. Int. J. Plast. 125, 169-190.

θ’ phase

Tetragonal lattice ($I\bar{4}m2$) with *a* = 4.05 Å and *c* = 5.80 Å

$(001)_{\theta'} || (001)_{Al}$ and $[100]_{\theta'} || [100]_{Al}$





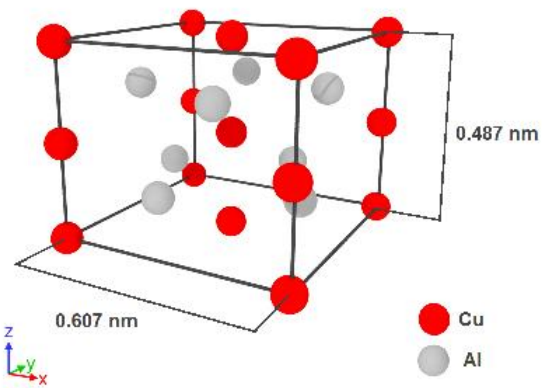
Krasnikov, V.S., Mayer, A.E., 2019. Int. J. Plast. 119, 21-42.

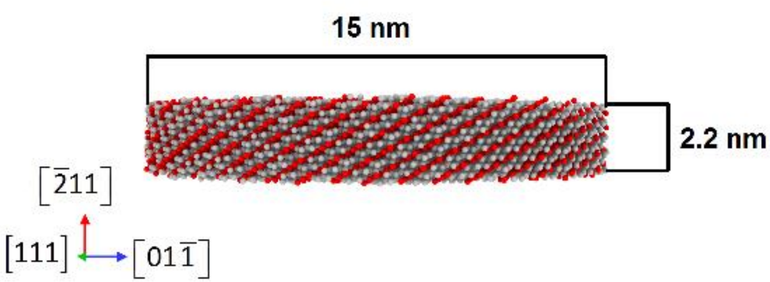
θ phase

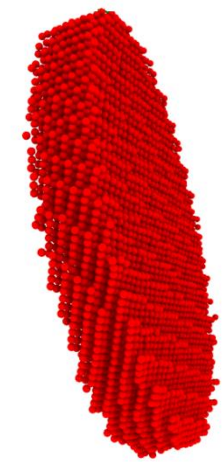
Tetragonal lattice (*I4mcm*) with a = 6.07 Å and c = 4.87 Å

$(\bar{1}\,2\,0)_\alpha \parallel (\bar{2}\,1\,1)_\theta$, $[2\,1\,1]_\alpha \parallel [1\,1\,1]_\theta$, Vaughan I orientation

(Vaughan and Silcock, 1967; Ringer et al., 1994)

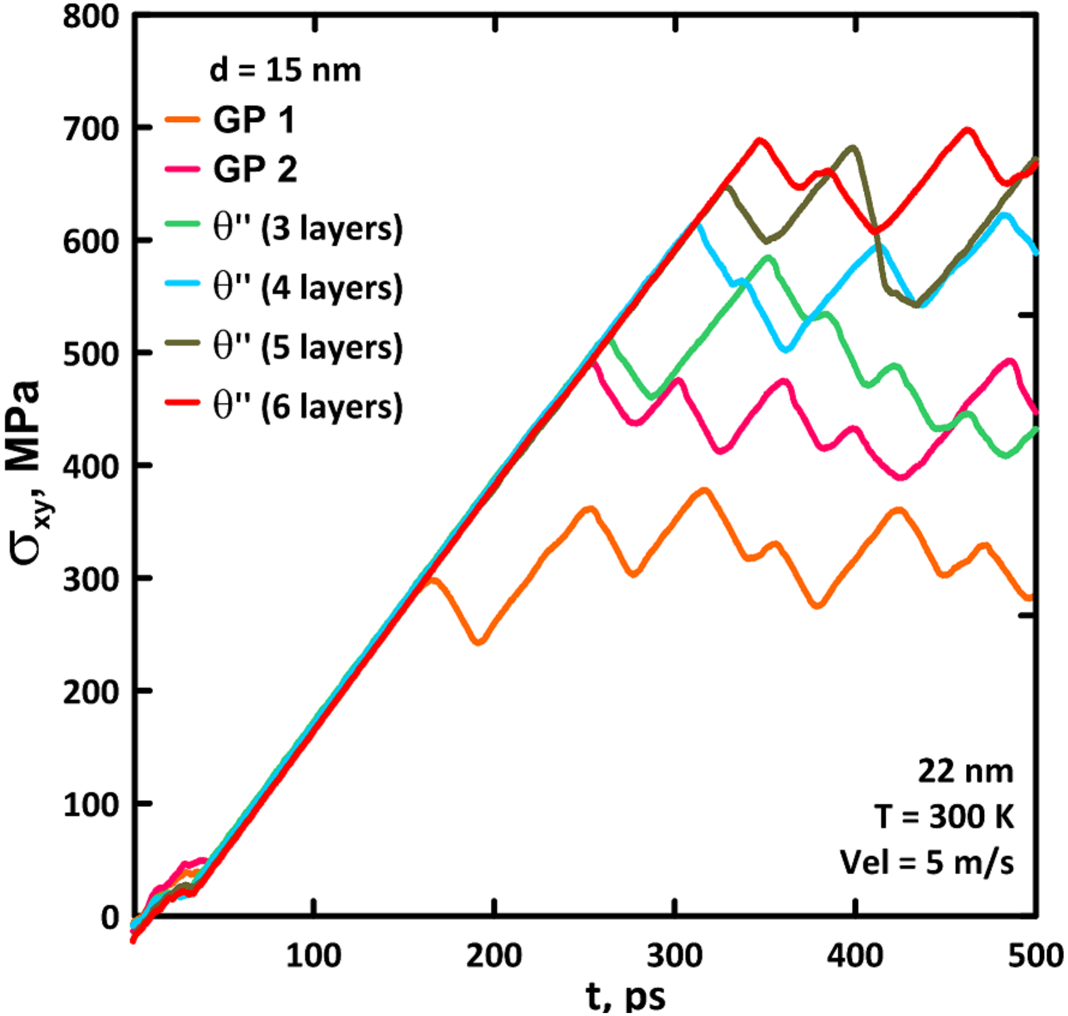






Krasnikov, V.S., Mayer, A.E., Pogorelko, V.V., 2020. Int. J. Plast. 128, 102672

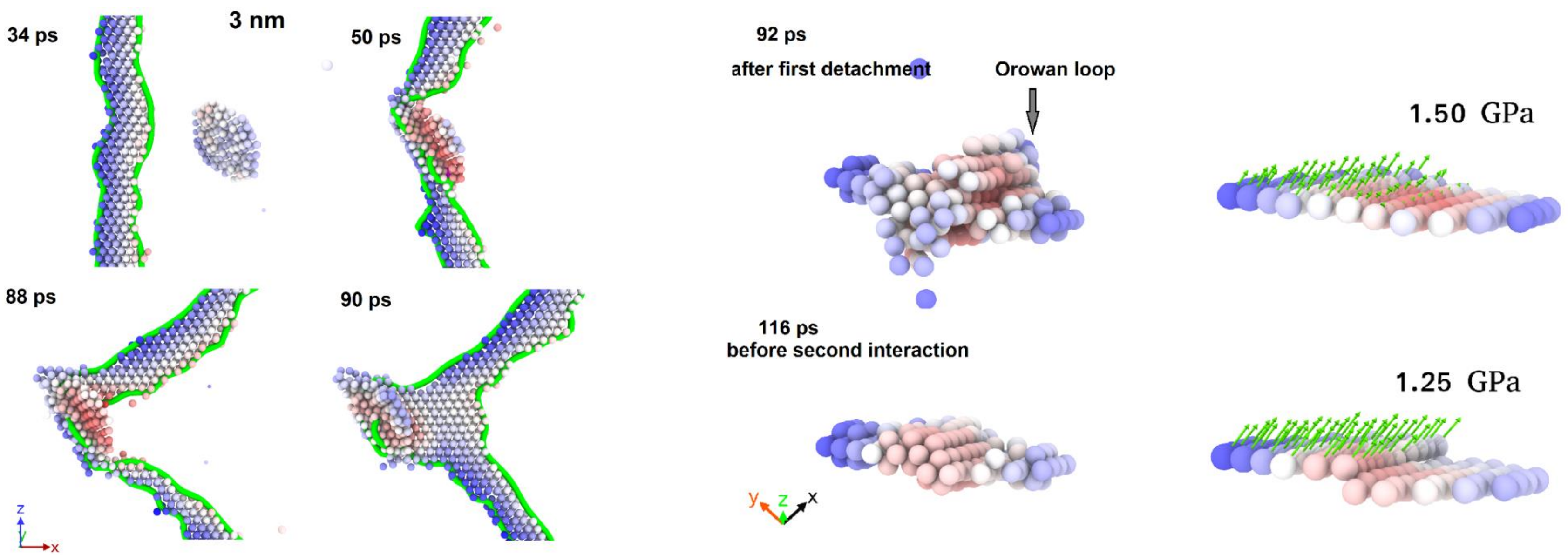
Stresses in MD system



Average stress in MD system with GP or θ''

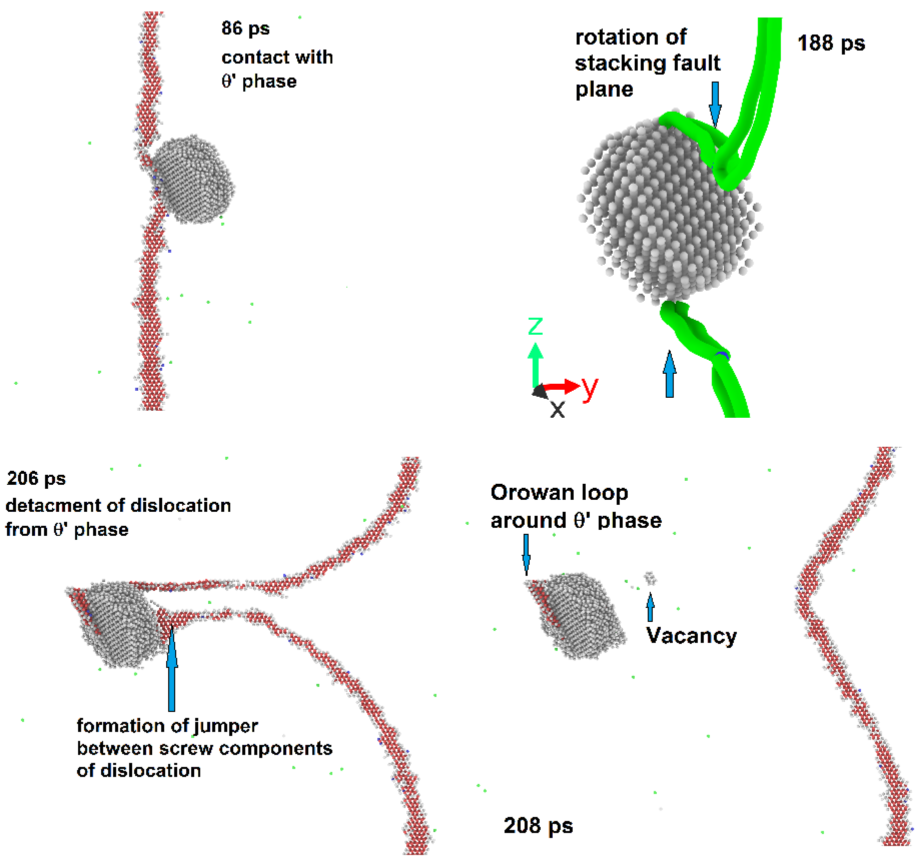
Mechanisms of dislocation-precipitate interaction

- Shearing of precipitates:
  - the smallest precipitates – GP_1 (less than 15 nm in diameter)



Mechanisms of dislocation-precipitate interaction

- Orowan looping around precipitates:

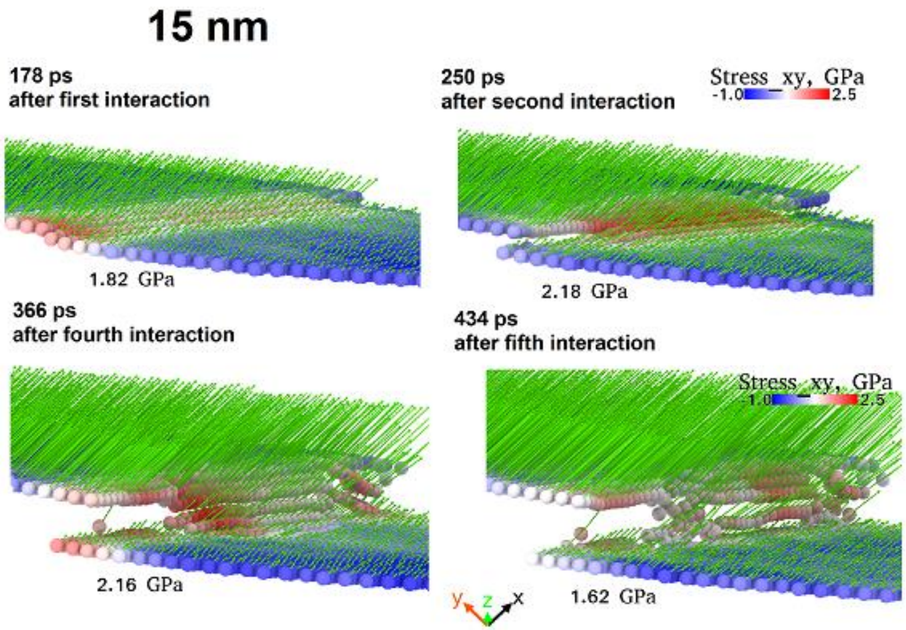


- screw character of elongated segments;
- activation of cross-slip;
- emission of vacancies after detachment.

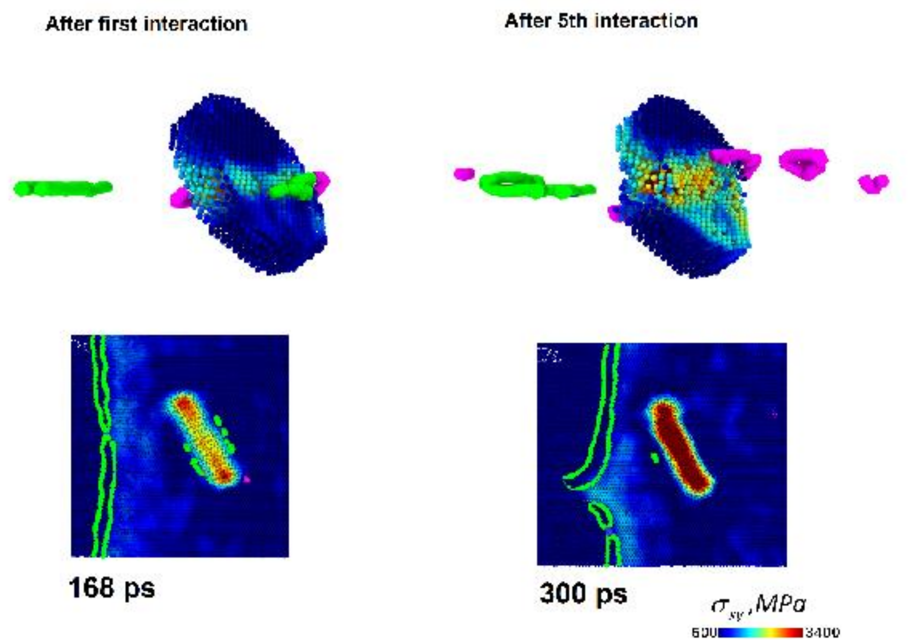
Mechanisms of dislocation-precipitate interaction

- Delayed shearing of precipitates

GP$_1$ zone of 5 nm

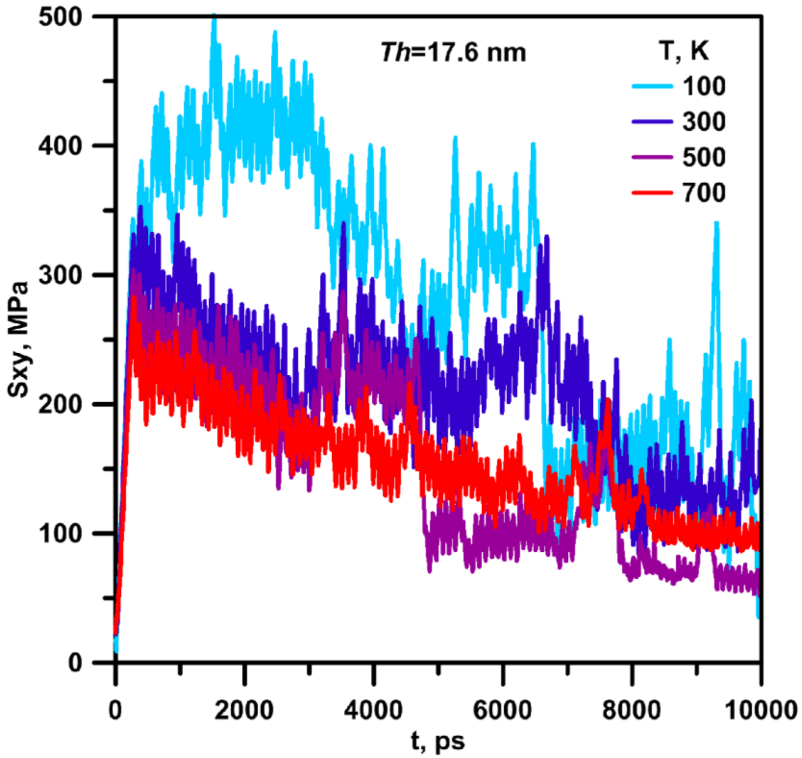


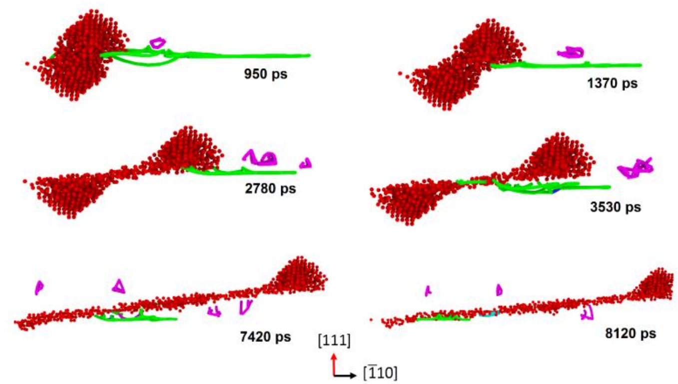
θ’ of 5 nm

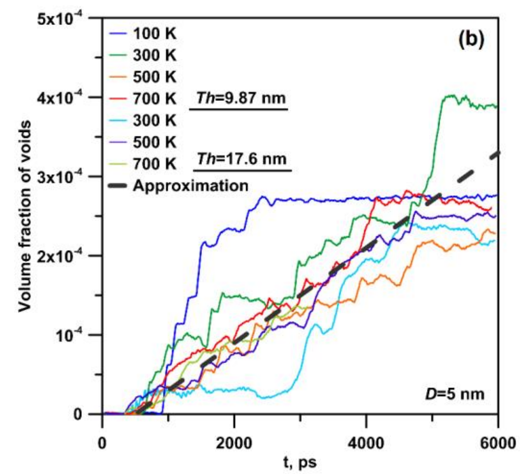


Prolonged plastic deformation

Average stress in MD system with θ', form of precipitate, and volume fraction of vacancies versus time.



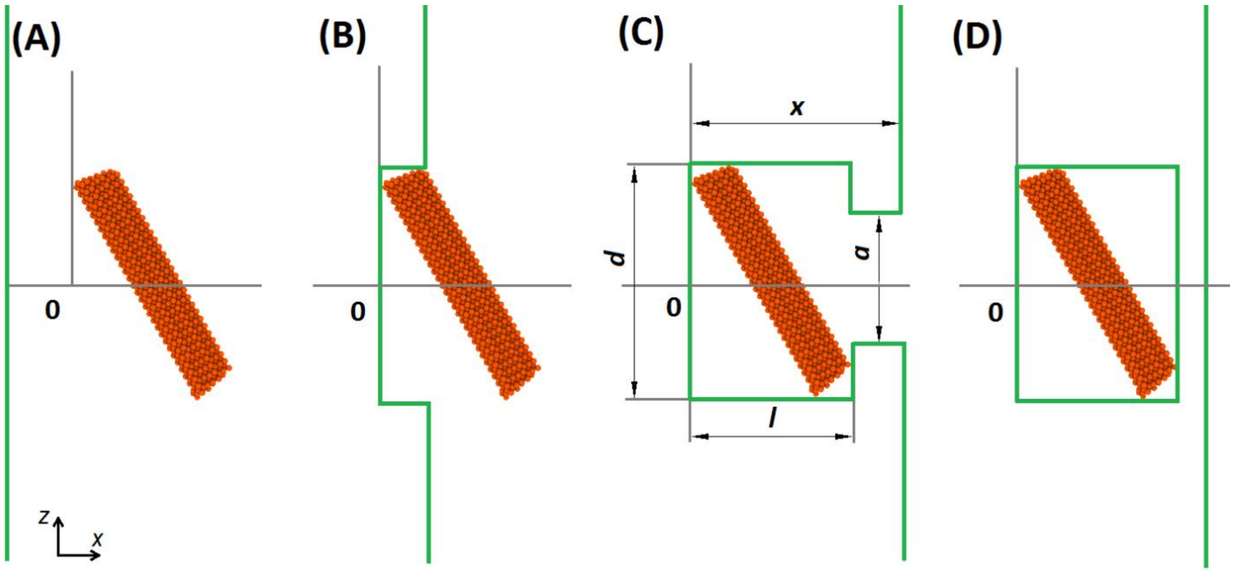




Shearing and even dissolution of θ' occur with plastic deformation in experiments (da Costa Teixeira et al., 2009; Murayama et al., 2001; Liu et al., 2011; Dobromyslov et al., 2012; Da-xiang et al., 2015; Olasumboye et al., 2018; Chung et al., 2018; Kaira et al., 2019; Azimi et al., 2019).

Accumulation of voids in shear bands is assumed to be the initiators of fracture of material (Olasumboye et al., 2018)

Model of dislocation-precipitate interaction



(A) – motion of dislocation in pure aluminum;
(B) – formation of additional segments with specific energy;
(C) – formation of jumper between elongated segments;
(D) – detachment of dislocation.

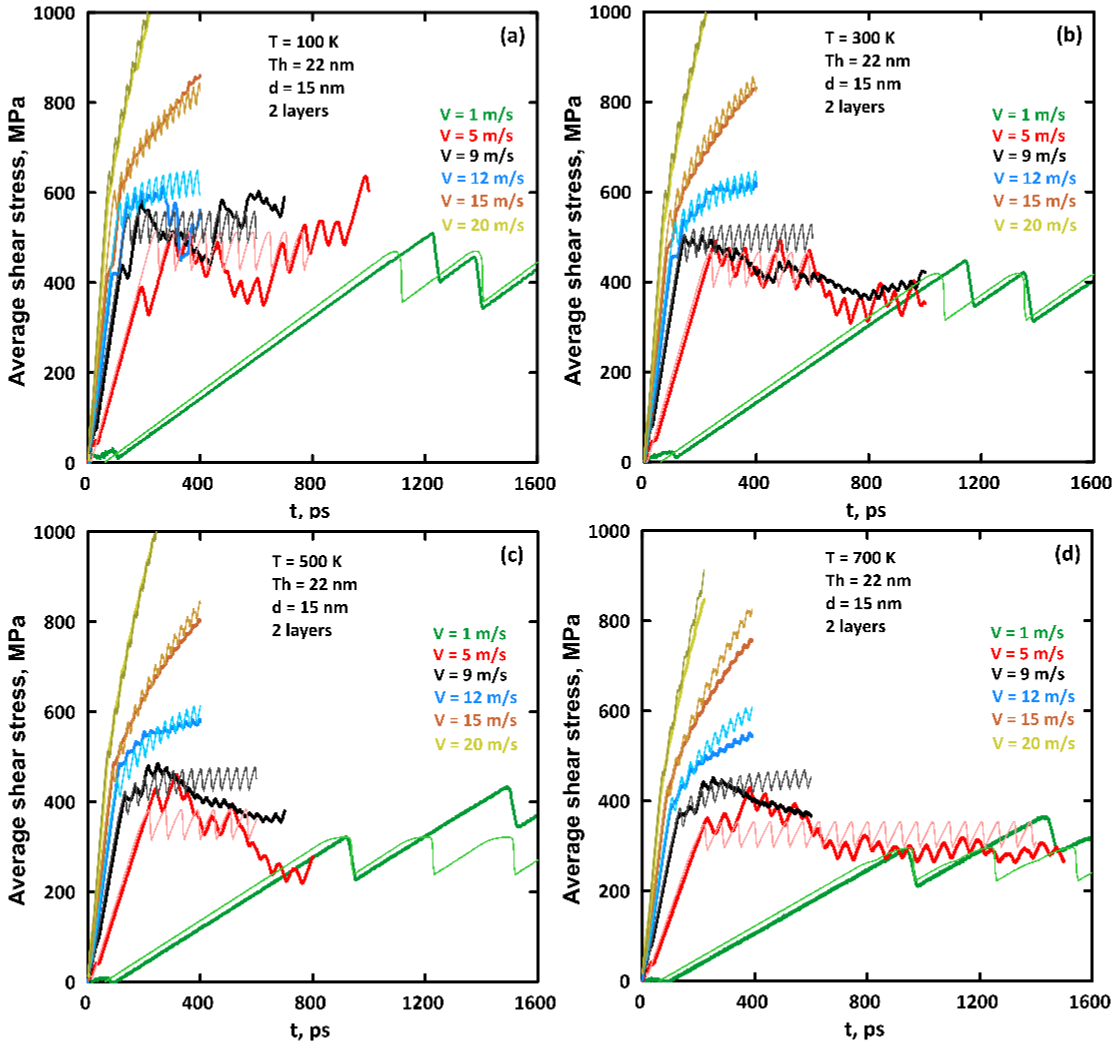
$$m_0 \ddot{x} = F_x \left(1 - \dot{x}^2 / c_t^2\right)^{3/2} - B_0 \dot{x},$$

$$F_x = -\frac{1}{L_x}\frac{\partial E_D}{\partial x},$$

$$E_D = -S_D b \sigma' + L_D \varepsilon_D .$$

Specific energies ε_D for additional segments are fitted from comparison with MD data for all studied precipitates.

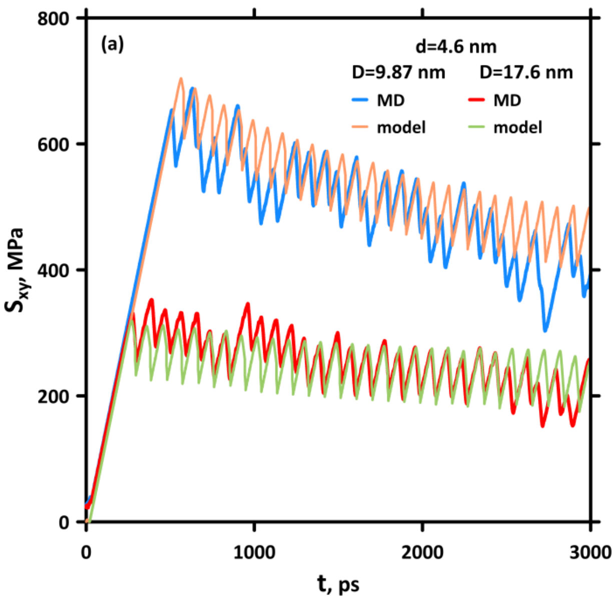
Model of dislocation-precipitate interaction

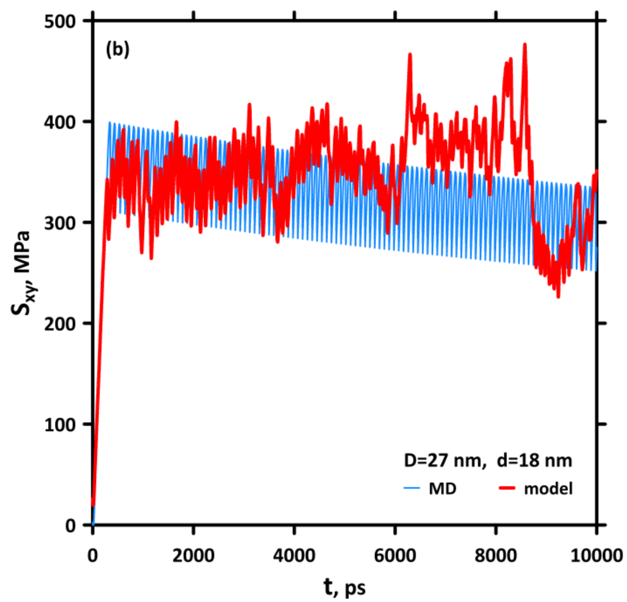


Average stress in systems with GP_2.

Comparison of MD data and interaction model predictions.

Model of dislocation-precipitate interaction





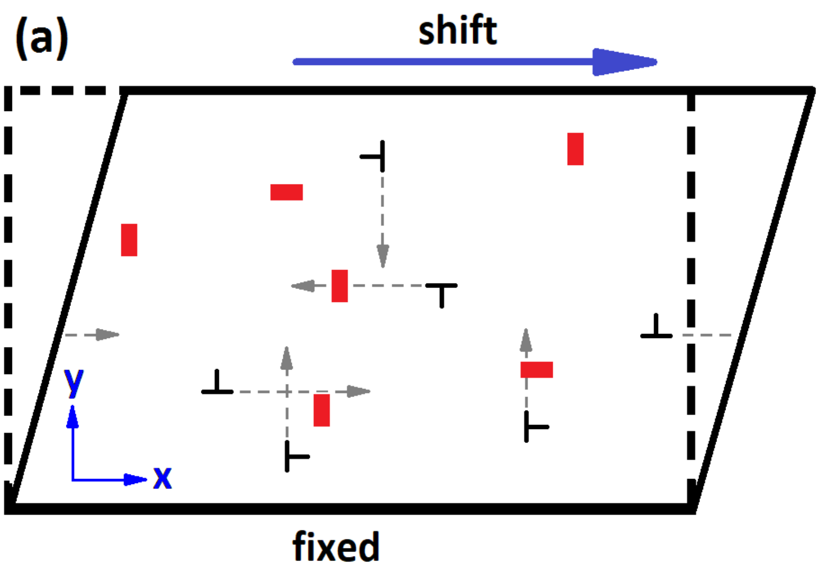
- Accounting of θ' precipitate softening

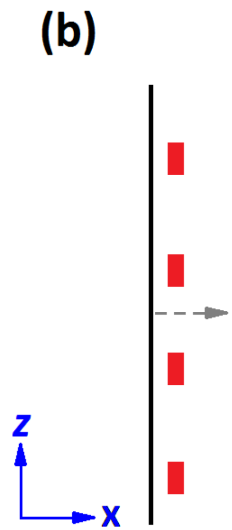
Average stress in system for different precipitate diameters *d* and different distances between the inclusions *D*. Comparison of the results of multiple interactions of the dislocation with θ' phase obtained by the model and MD

$$d = d_0 \exp\left[-k(d_0)N\right], \qquad k(d_0) = 0.084 \cdot \exp\left[-d_0 \cdot 0.224\ \mathrm{nm}^{-1}\right]$$

θ' of 60 nm and larger are stabile (Kaira et al., 2019).

Discrete dislocation dynamics





2D approach

Log-normal distribution over precipitate diameter

$$\frac{\Delta N}{\Delta d} = \frac{1}{\sqrt{2\pi\sigma\mu d}} \exp\left[-\frac{(\ln(d)-\mu)^2}{2\sigma^2\mu^2}\right]$$

$$\sigma_{xy} = 2G\left(u_{xy} - w_{xy}\right)$$

$$\sigma_{xx} = 2G\left[u_{xx} - \left(u_{xx}+u_{yy}\right)/3 - w_{xx}\right] + K\left(u_{xx}+u_{yy}\right)$$

$$\sigma_{yy} = 2G\left[u_{yy} - \left(u_{xx}+u_{yy}\right)/3 - w_{yy}\right] + K\left(u_{xx}+u_{yy}\right)$$

$$\rho\frac{d^2u_x}{dt^2} = \frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}$$

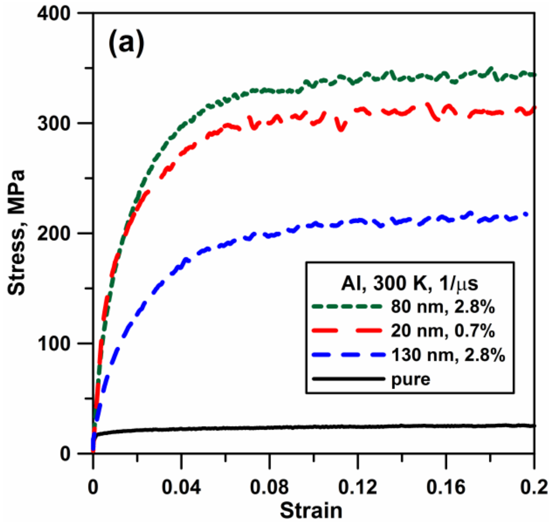
$$\rho\frac{d^2u_y}{dt^2} = \frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}$$

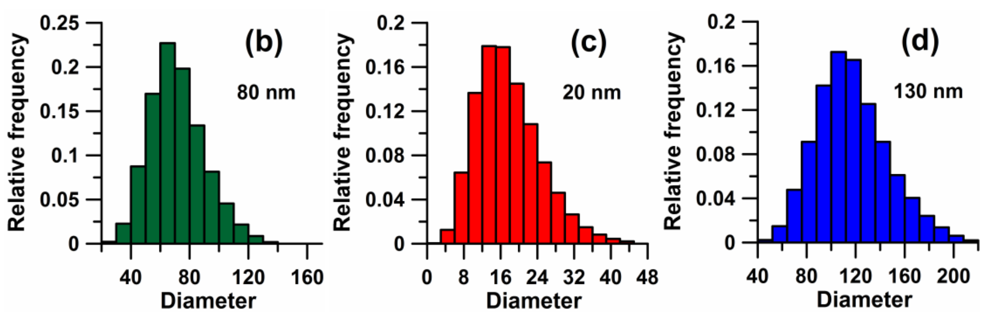
$$w_{\alpha\beta} = \frac{1}{2}\sum_{k=1}^{N_D}\left(n_\alpha^{(k)}b_\beta^{(k)} + n_\beta^{(k)}b_\alpha^{(k)}\right)v^{(k)}\delta\left(l^{(k)}\right)$$

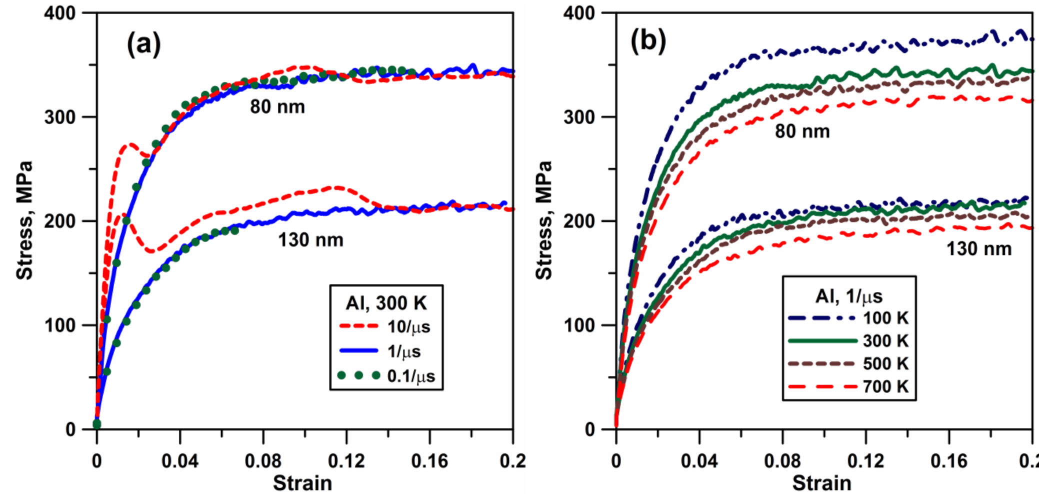
+ model of dislocation-precipitate interaction

Discrete dislocation dynamics

Stress-strain curves for pure aluminum and three alloys







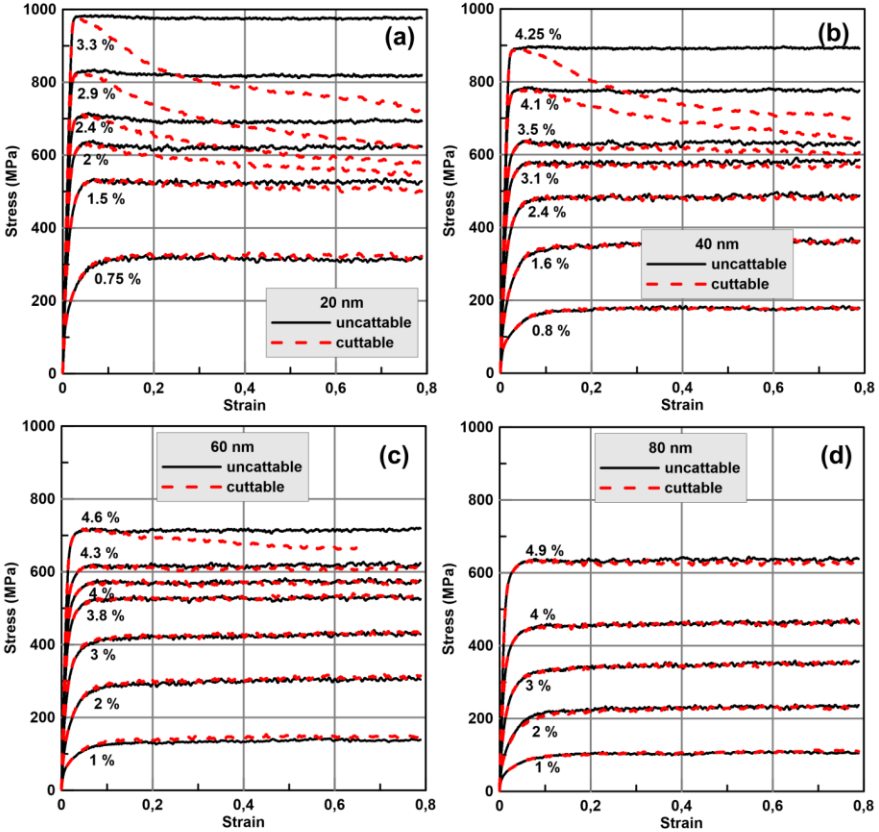
(a) strain rate and (b) temperature sensitivities for two alloys

Experimental data for Al alloys

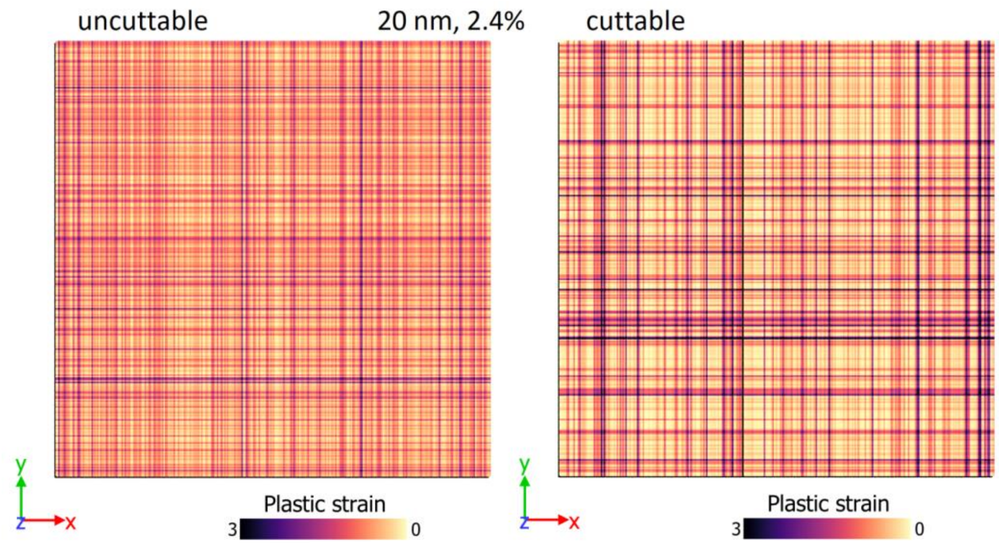
Work	Al alloy	$\dot{\varepsilon}$, s^{-1}	σ_{YS}, MPa
Elkhodary et al., 2009	2139-T8	$10^3 – 10^4$	820
Casem and Dandekar, 2012	2139-T8	$2 \cdot 10^3$	540
Da-xiang et al., 2015	2519-T8 and T9	$10^3 – 10^4$	470 – 500
Liu et al., 2016	7055-T7	$6 \cdot 10^3$	605
Cao et al., 2018	2139-T8	$7.5 \cdot 10^3$	580
Edwards et al., 2019	2024-T351	$5 \cdot 10^3 – 2 \cdot 10^4$	215 (RSS)

Discrete dislocation dynamics

Stress-strain curves for four alloys



- Accounting of precipitate softening

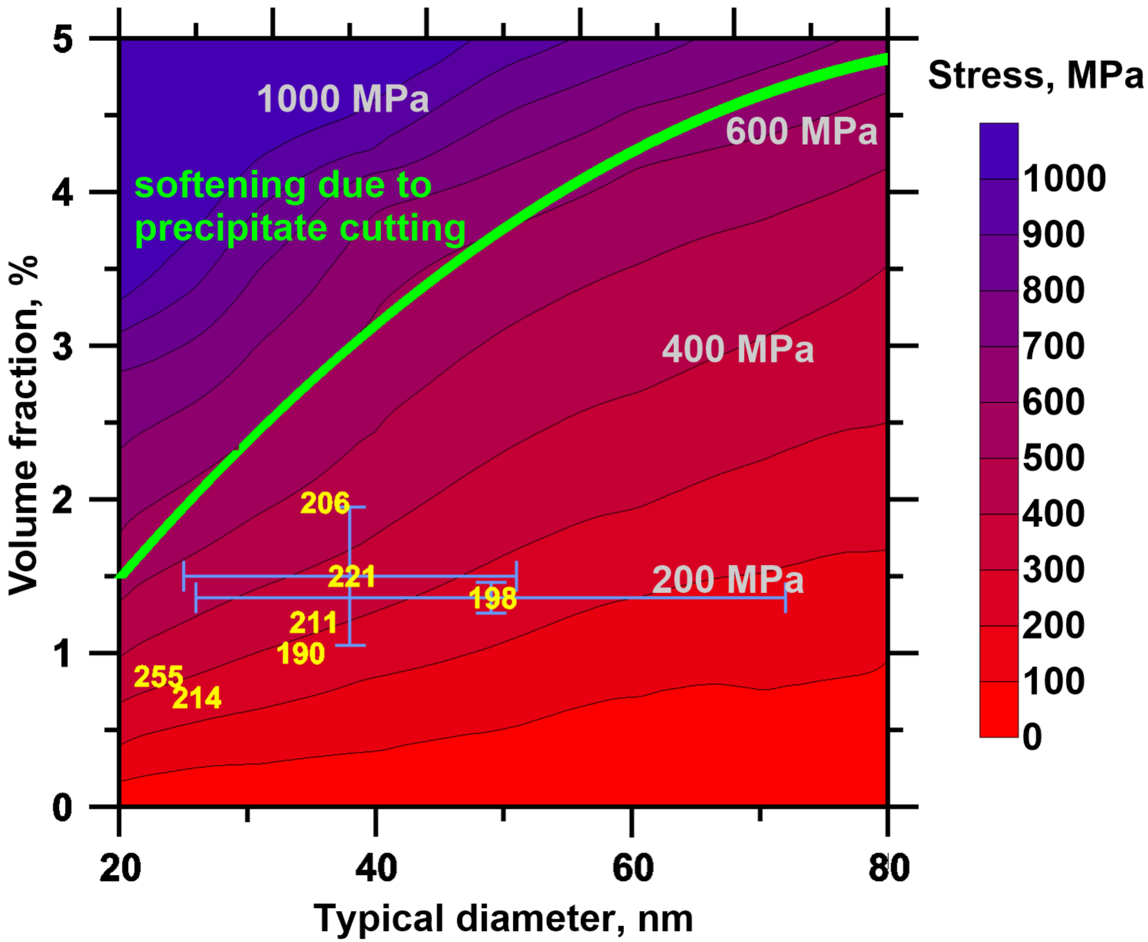


Distribution of plastic deformation

Presence of cut precipitates in alloy leads to decrease in the strain hardening rate (Deschamps et al., 2013).

(Gazizov and Kaibyshev, 2016) observed softening of AA2139; this softening due to repeated cutting of Ω phases.

Discrete dislocation dynamics



Accounting of precipitate cutting allows to select the region where softening of alloys is possible

Experimental data from (Zuiko and Kaibyshev, 2020).

Conclusions

- Mechanism of dislocation-precipitate interaction in Al-Cu system has complex character;
- Prolonged plastic deformation provokes decrease of precipitate strength;
- Dislocation-precipitate interaction model is offered and fitted on MD data;
- 2D discrete dislocation dynamics is realized with dislocation-precipitate interactions, precipitate statistics and precipitate softening;
- DDD adequately predicts flow stress and temperature softening of Al alloys;
- Existence of range of concentrations and sizes of precipitates is predicted, where decrease of precipitate contribution into alloy strength can occur.

Thank you for your attention!