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Shock induced plasticity in Al, Cu and Al-Cu alloys.

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Physics and Technology

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- Homogeneous nucleation
  - Mechanism
  - Energy of nuclei
  - Nucleation rate
- Mobility of single dislocation
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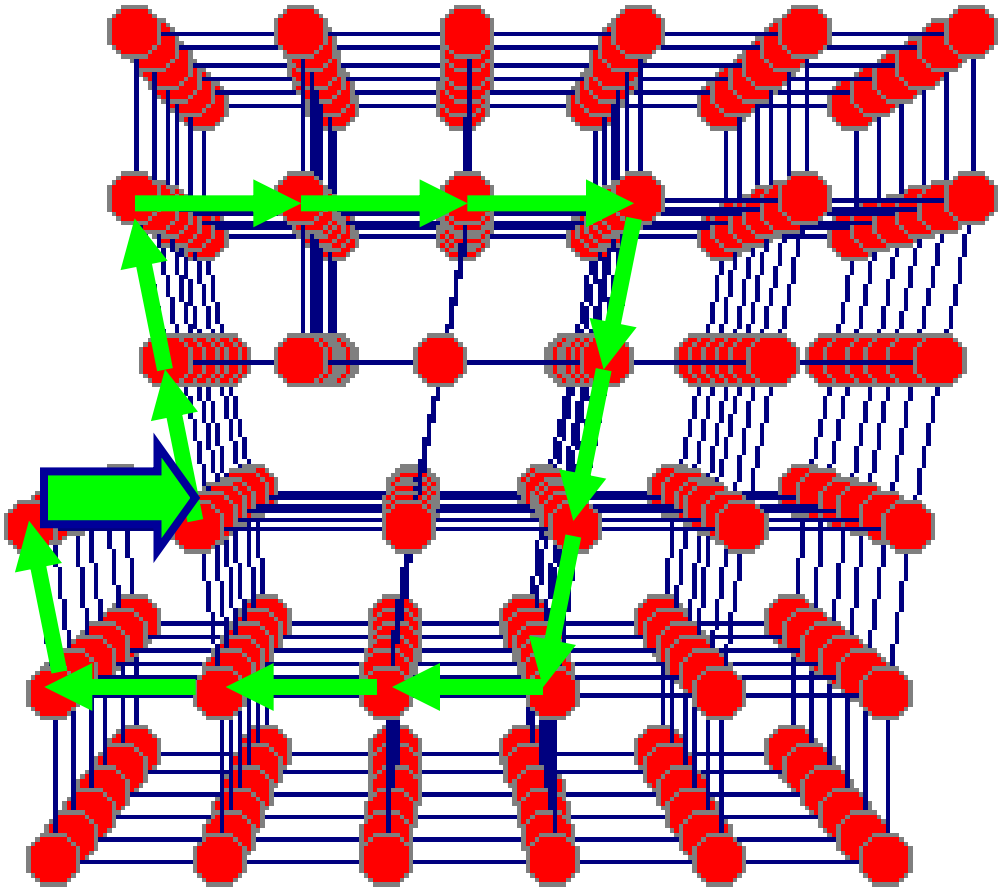
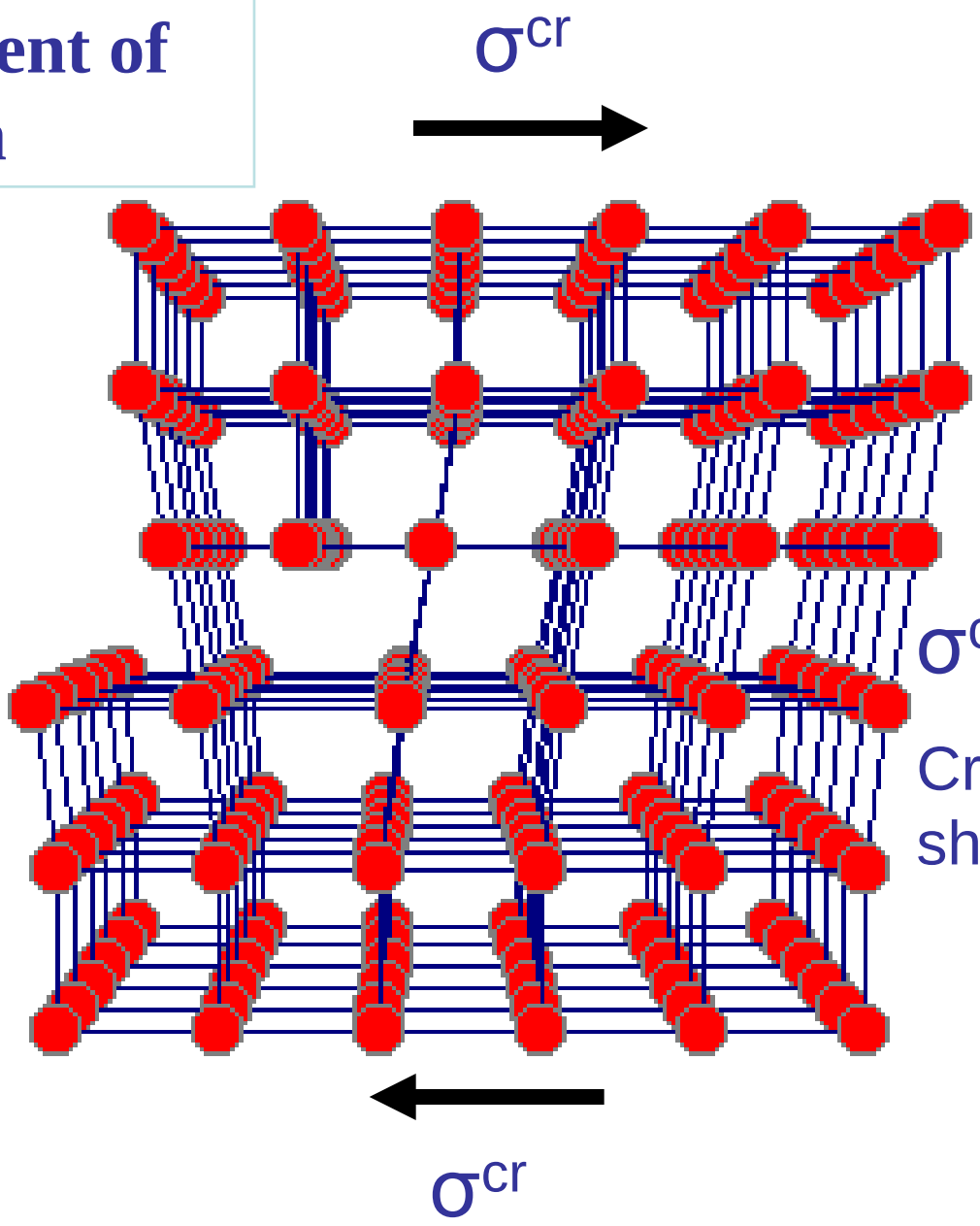
  - Dynamic yield stress in single crystals
- Dislocation interaction with obstacles
- Implementation of MD results in continuum model
  - Application to modeling of shock waves
- Conclusions

Edge dislocation

Burgers vector *b*

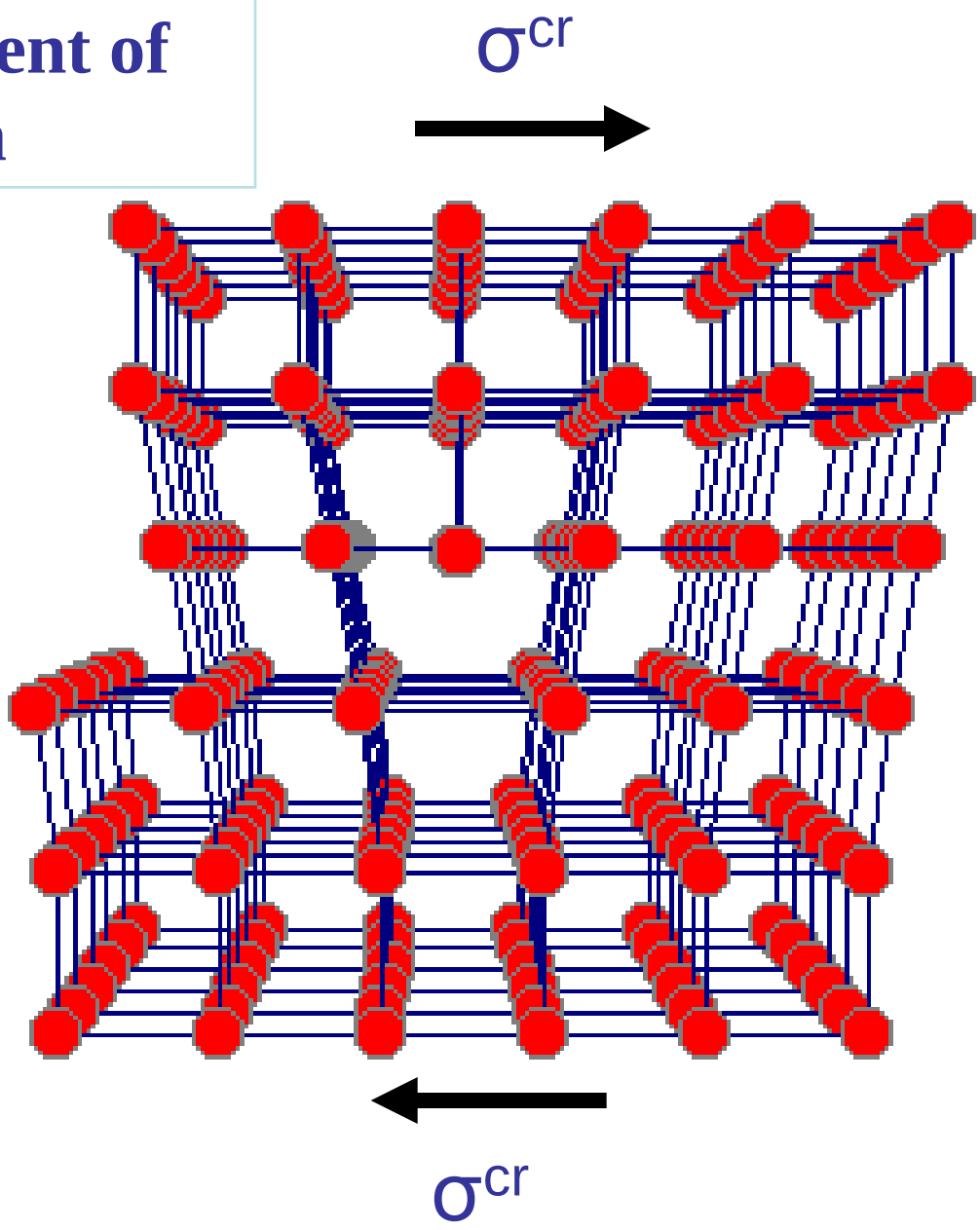


Displacement of dislocation

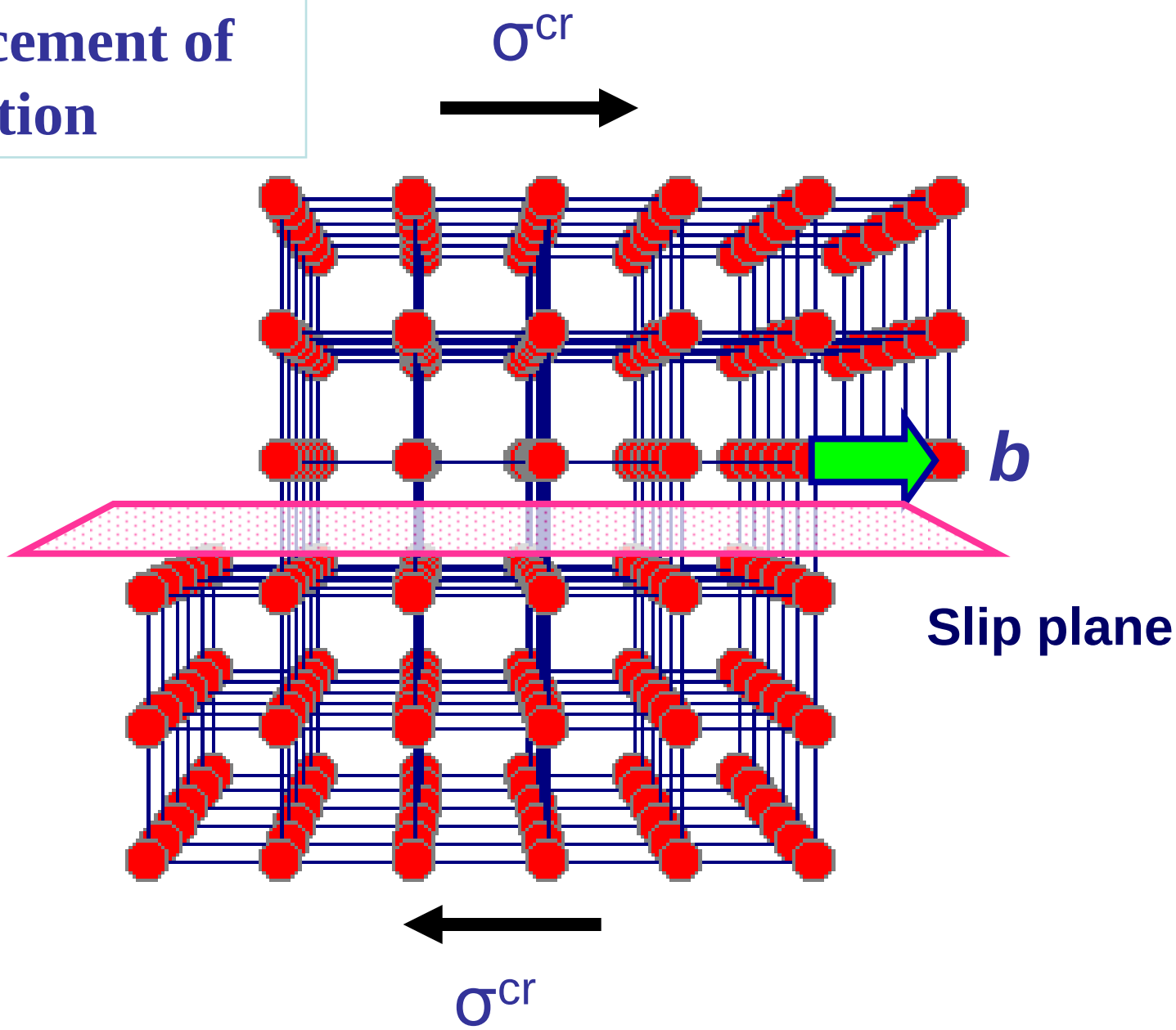


σ^{cr} – Critical value of shear stress

Displacement of dislocation



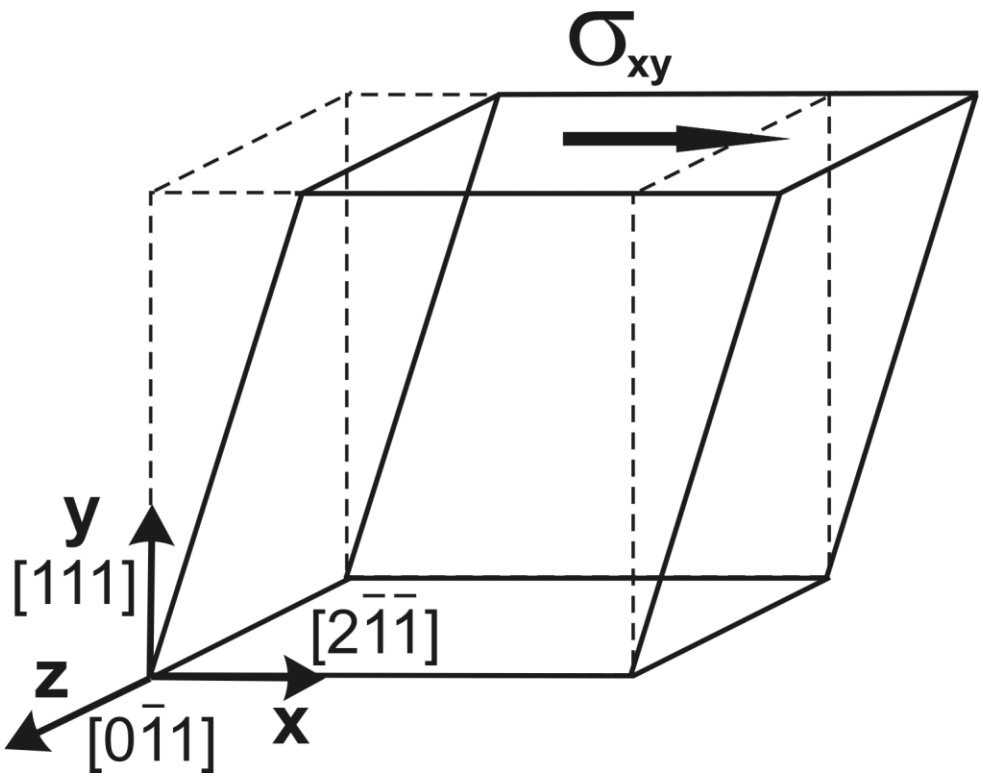
Displacement of dislocation



Homogeneous nucleation

MD model

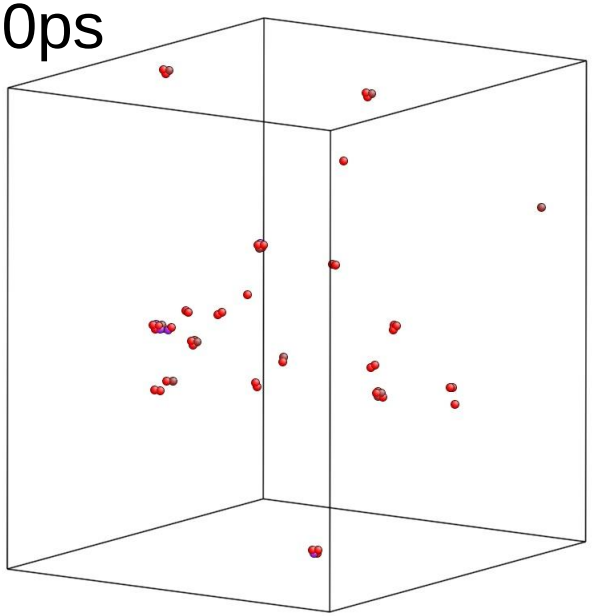
Ercolessi EAM potential for Al



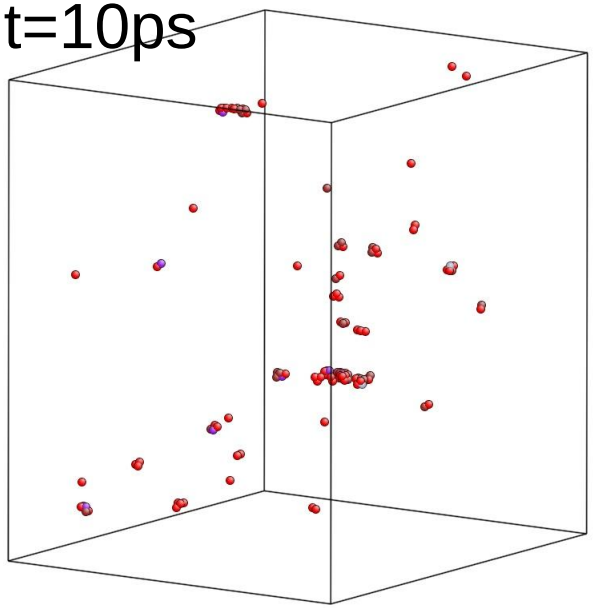
1. Shear deformation
2. Stress relaxation at fixed shear strain

Визуализация процессов зарождения

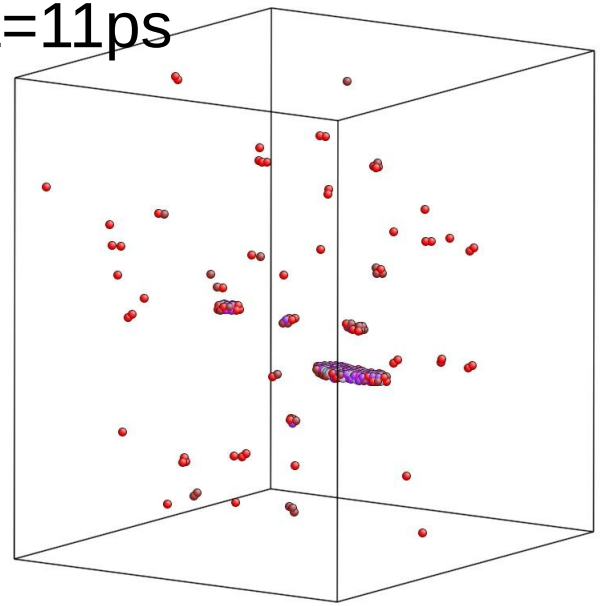
t=0ps



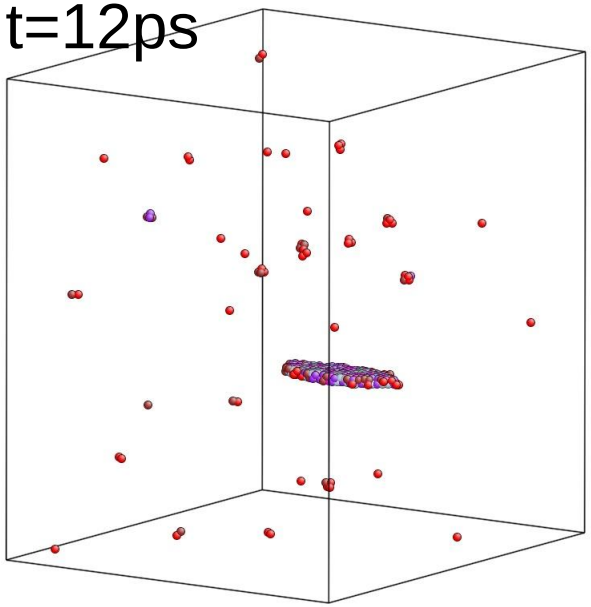
t=10ps



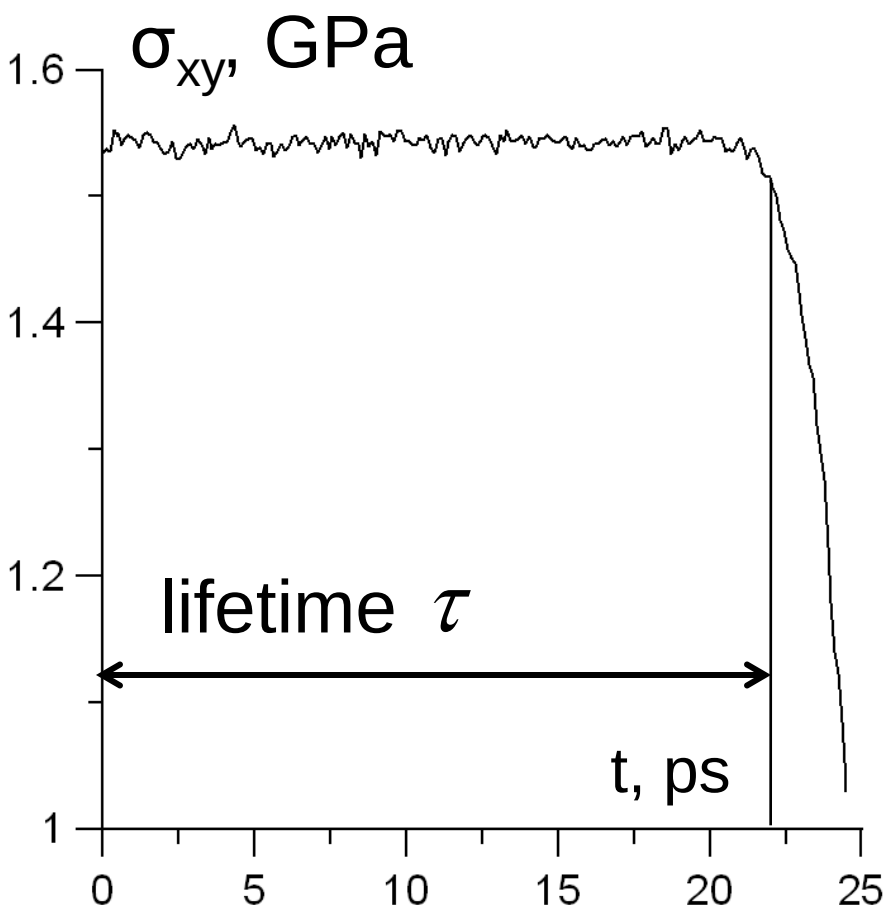
t=11ps

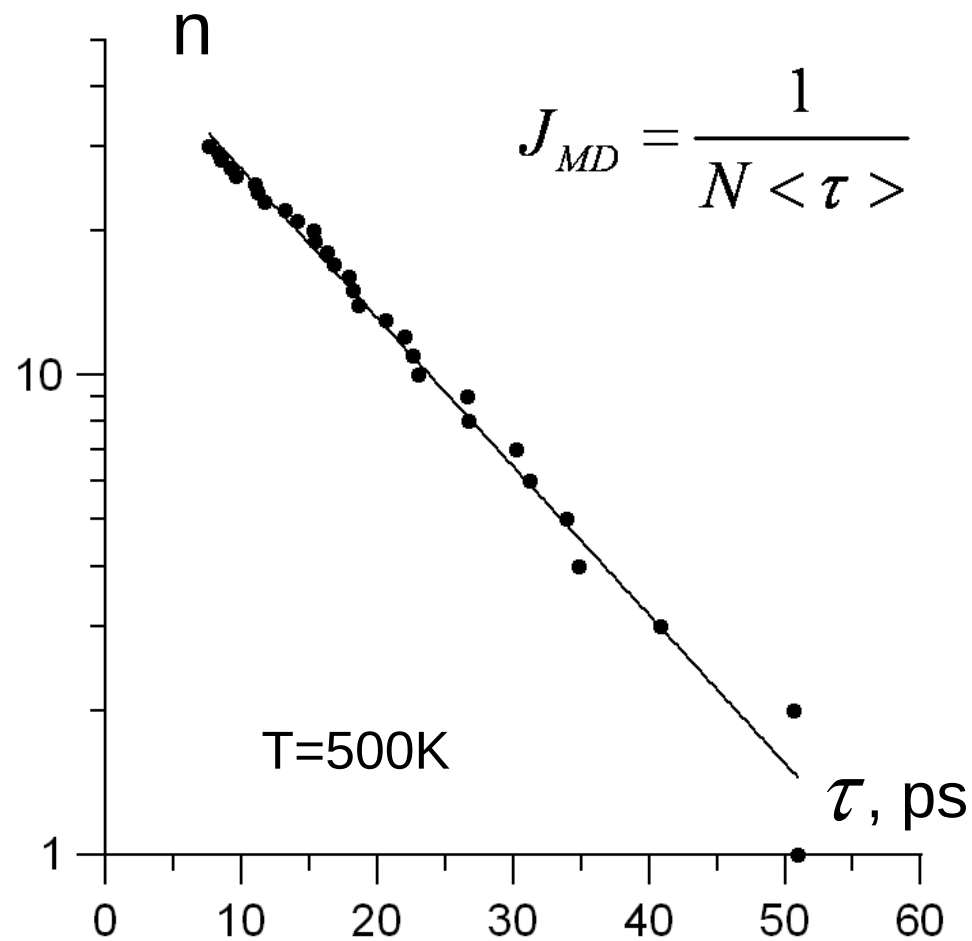


t=12ps



Stress relaxation and lifetime distribution

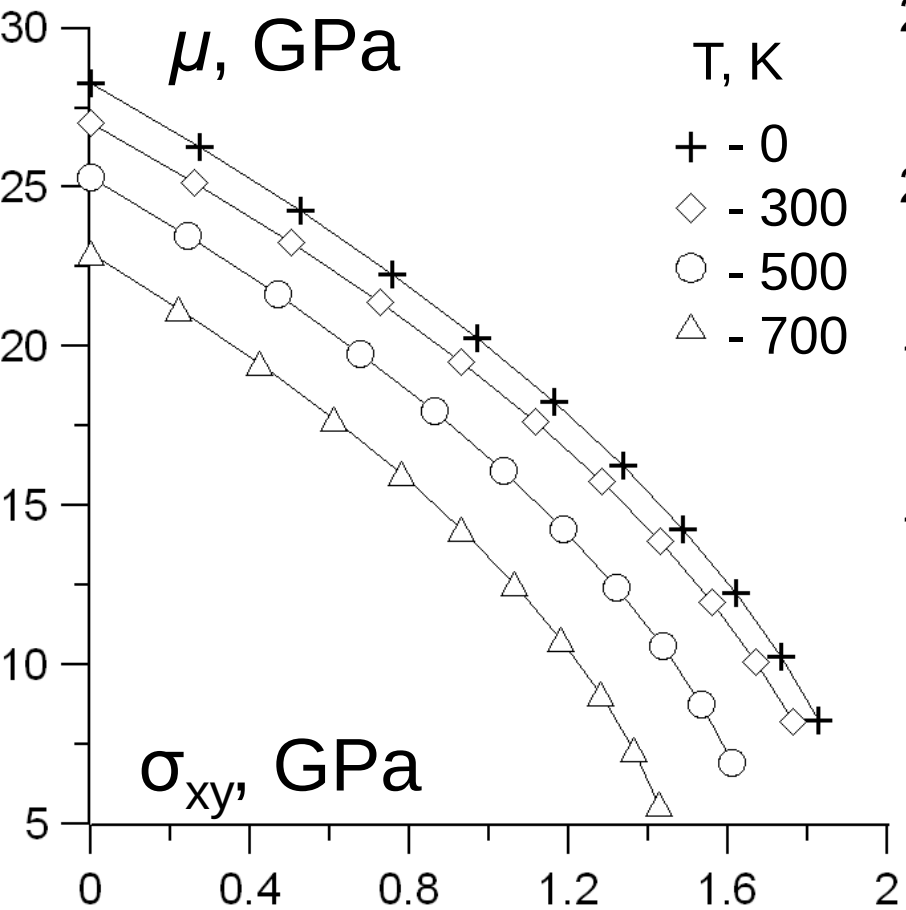


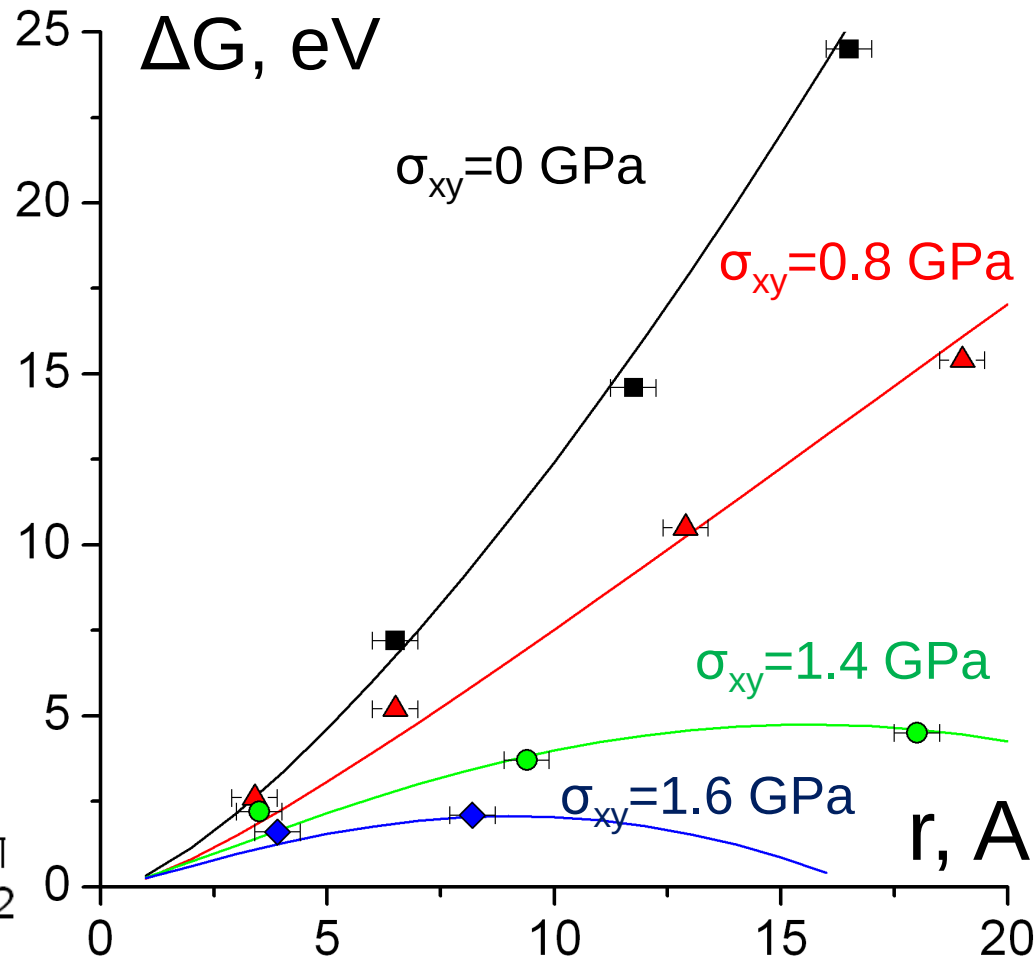


Energy of dislocation loop formation

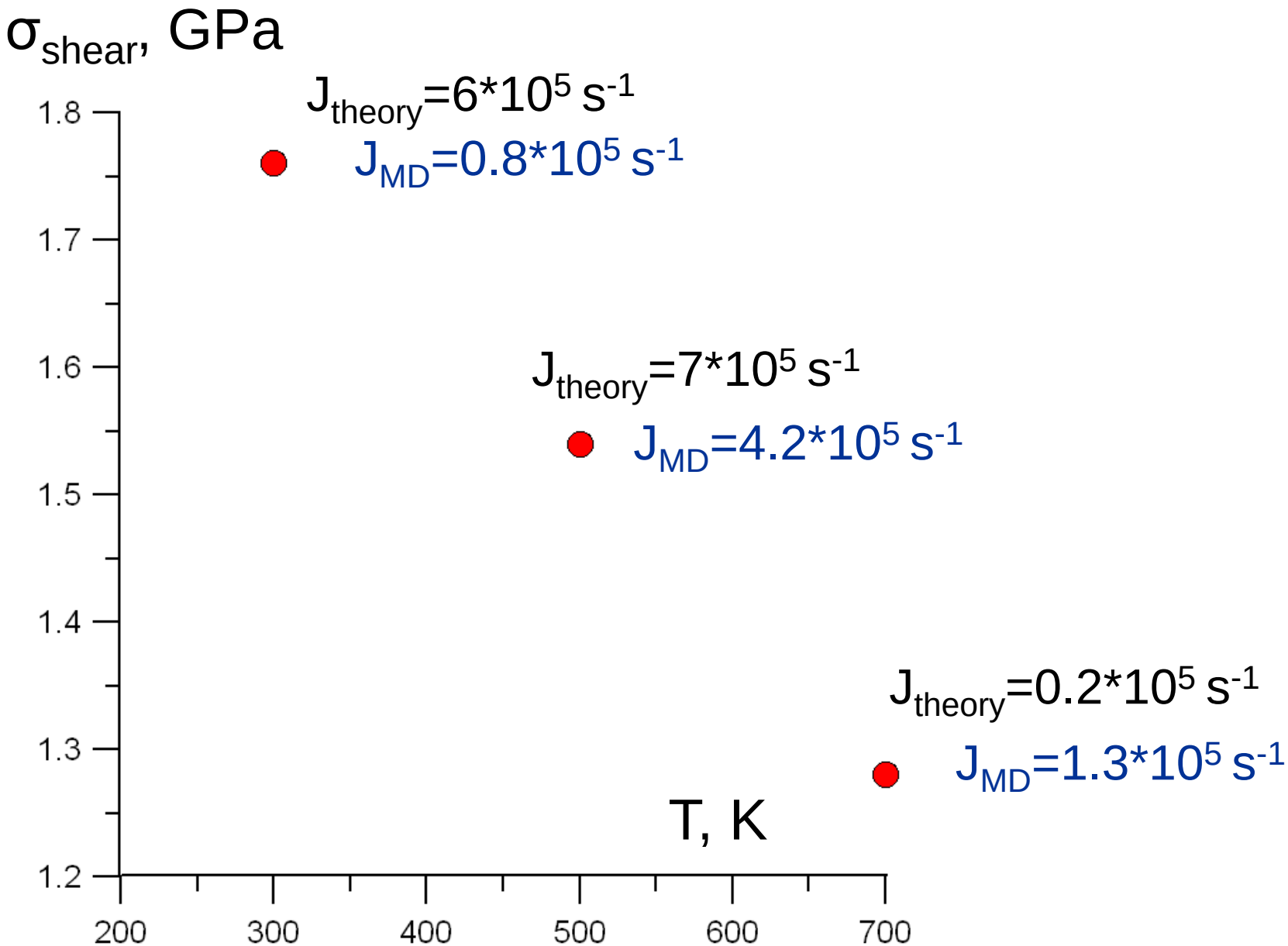
$$\Delta G = \boxed{2\pi r \frac{2-\nu}{2(1-\nu)} \frac{\mu b^2}{4\pi}\left[\ln\left(\frac{4r}{\rho}\right)-2\right]} - \boxed{\pi r^2 b\sigma} + \boxed{\pi r^2 \gamma}$$

dislocation loop energy relaxation stacking faults



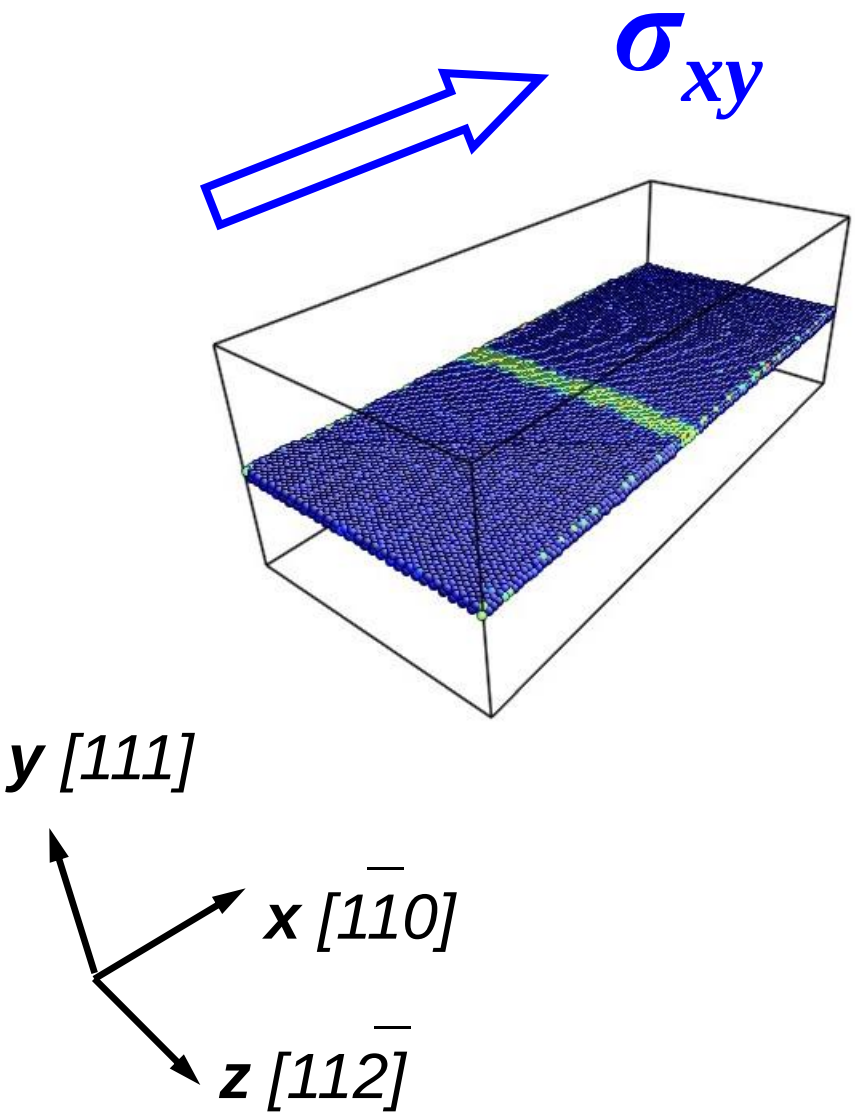


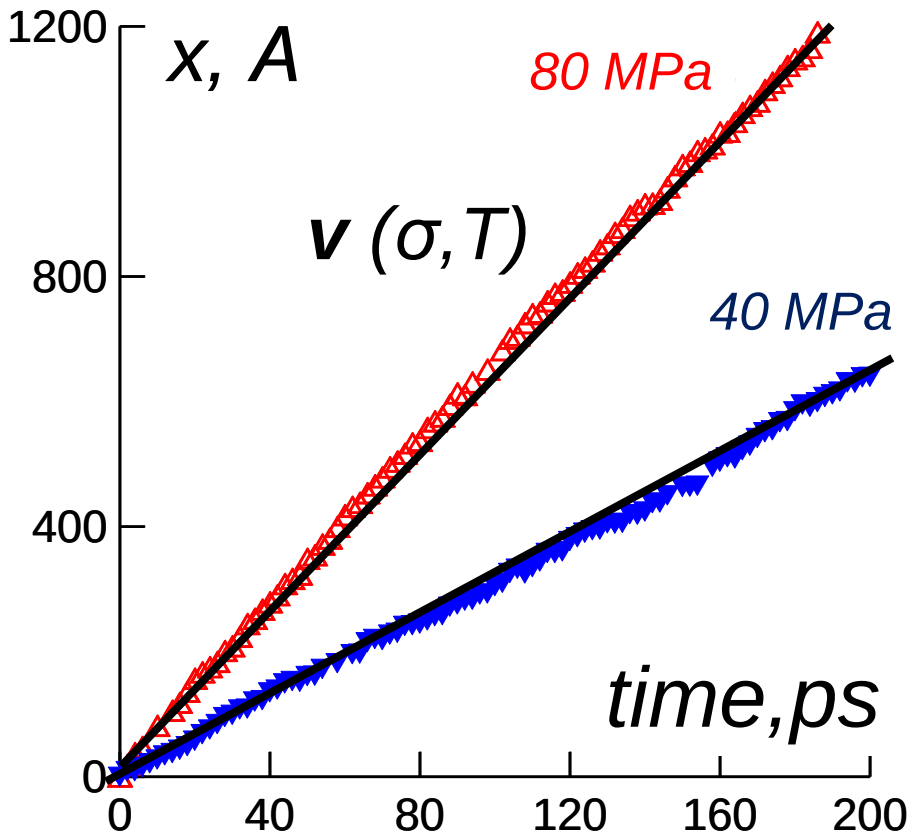
Nucleation rate: MD vs Dislocation Theory



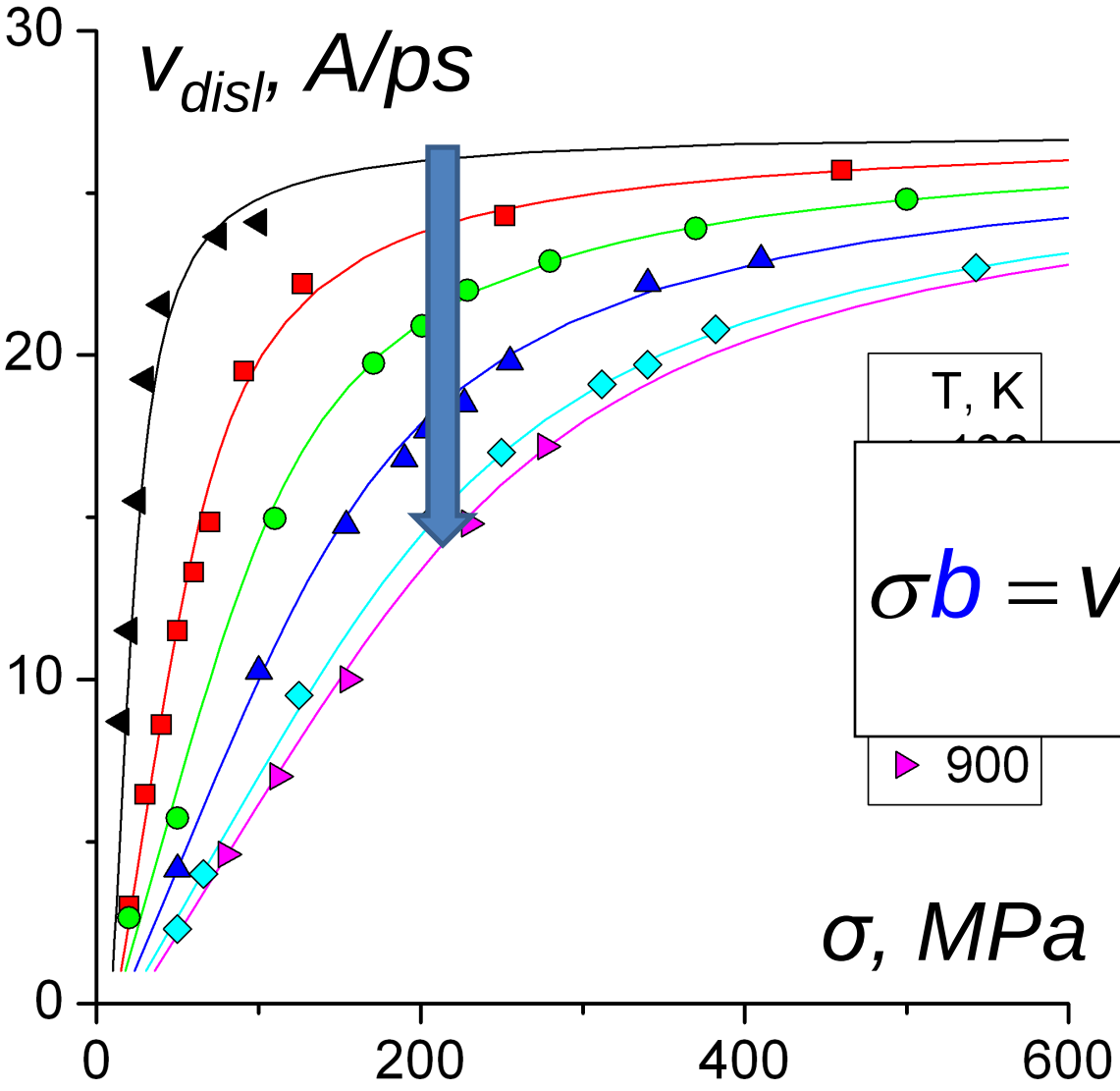
Dislocation motion

Steady-state dislocation motion during application of a shear stress





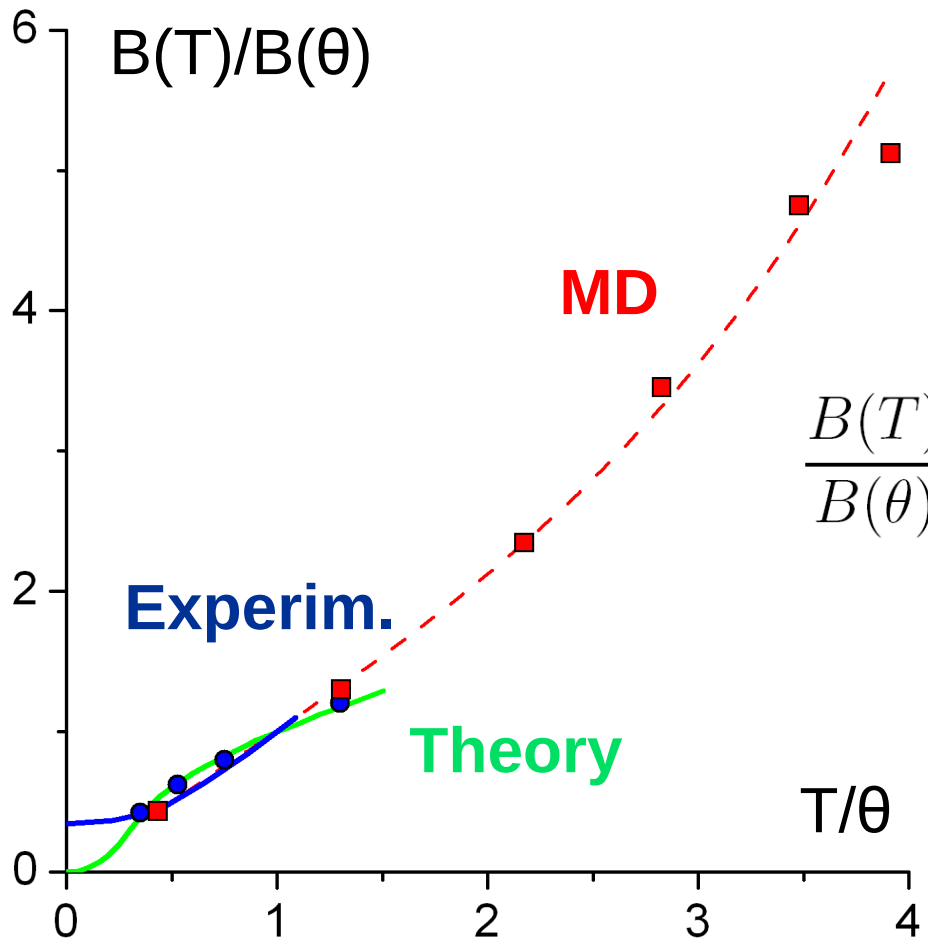
Phonon drag on dislocation



$$\sigma b = v_{disl} \frac{B_0(T)}{1-(v_{disl}/c)^4}$$

Temperature dependence of the drag coefficient B(T)

(θ=230 K)



$$\frac{B(T)}{B(\theta)} = \frac{T}{\theta} + 0.0077\left(\frac{T}{\theta}\right)^4$$

Near T ≈ 300 K :

0.9 x 10^{-5} Pa·s	MD, this work
0.5 x 10^{-5} Pa·s	ultrasound attenuation, 1970
2.6 x 10^{-5} Pa·s	dislocation mobility, 1969
17 x 10^{-5} Pa·s	ultrasound attenuation, 1966

Dynamic yield stress in single crystals

$$\dot{\varepsilon} \simeq 10^6 s^{-1}$$

$$b \simeq 2 \times 10^{-10} m$$

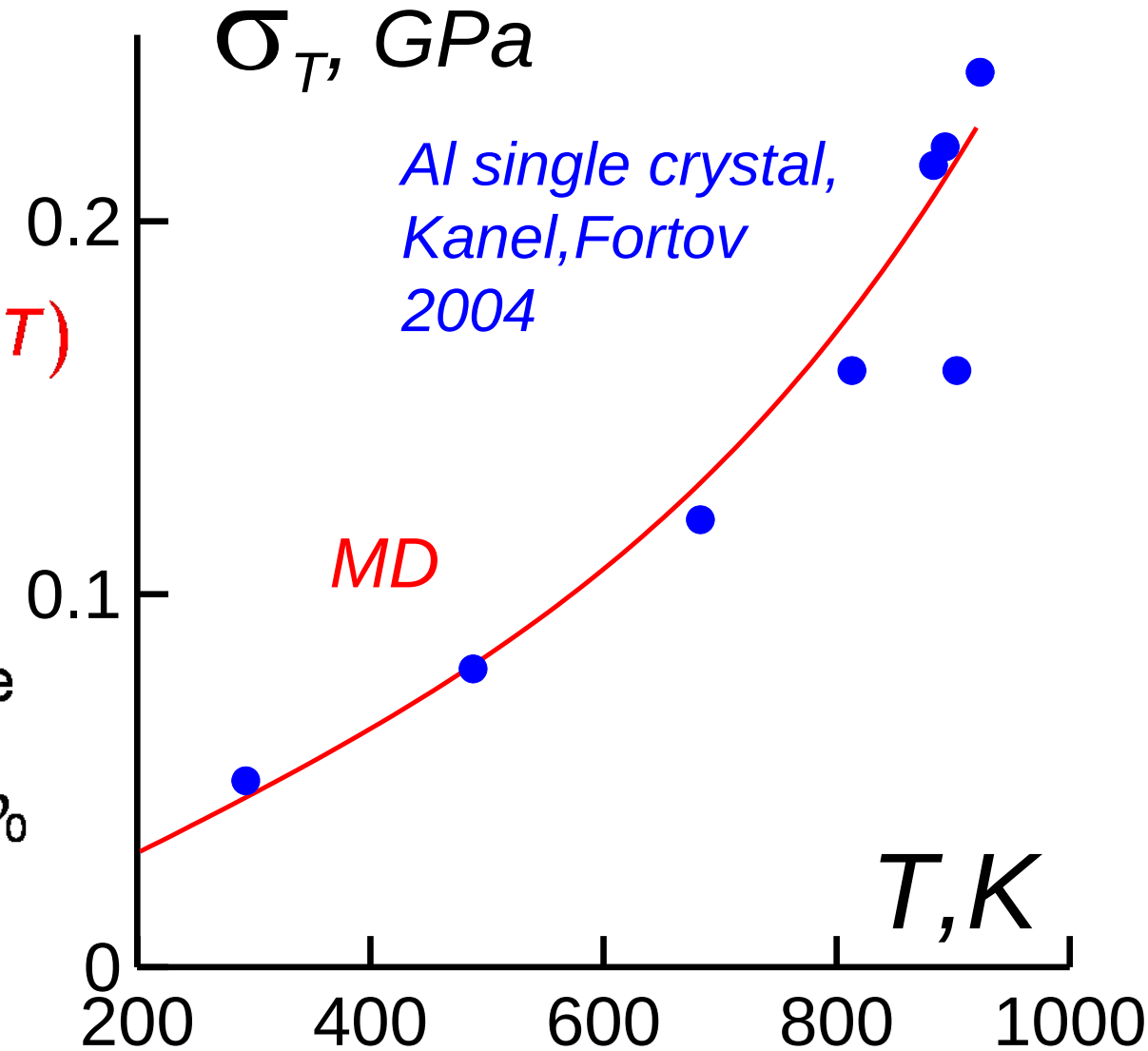
$$\sigma_T(T) = \frac{\dot{\varepsilon}}{\rho(T) b^2} B(T)$$

$$\rho \simeq 7 \times 10^8 cm^{-2}$$

Frank-Read source

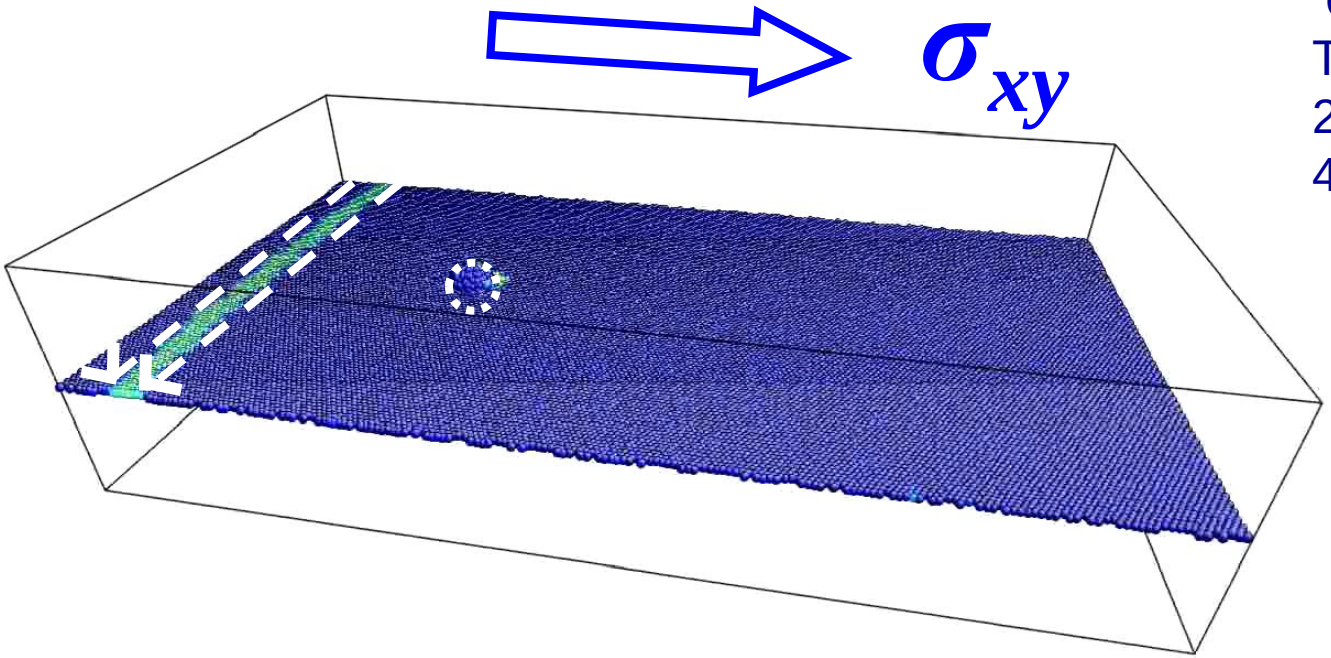
$$\rho \simeq \frac{\nu \cdot \tau}{L} \rho_0 \simeq 10^2 \rho_0$$

$$\rho \simeq 10^8 - 10^9 cm^{-2}$$

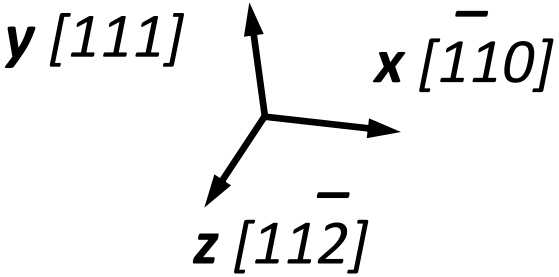


Dislocation interaction with precipitates and nanovoids

Interaction of dislocation with precipitates and voids

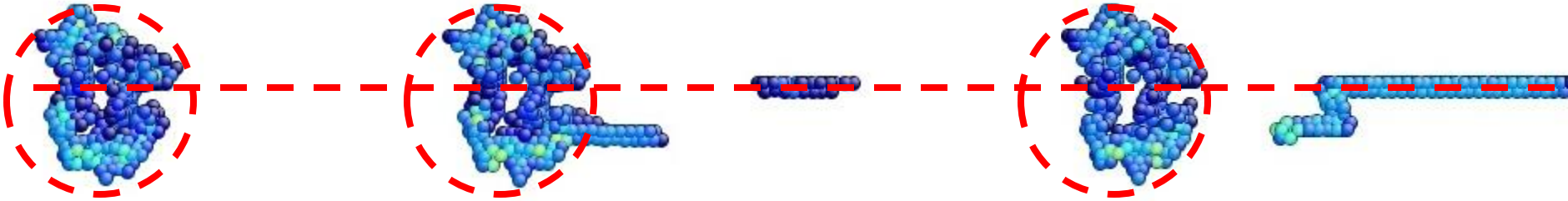


Cu cluster in Al
T=700 K,
20 x 4ps = 80ps
400Å x 80Å x 120Å

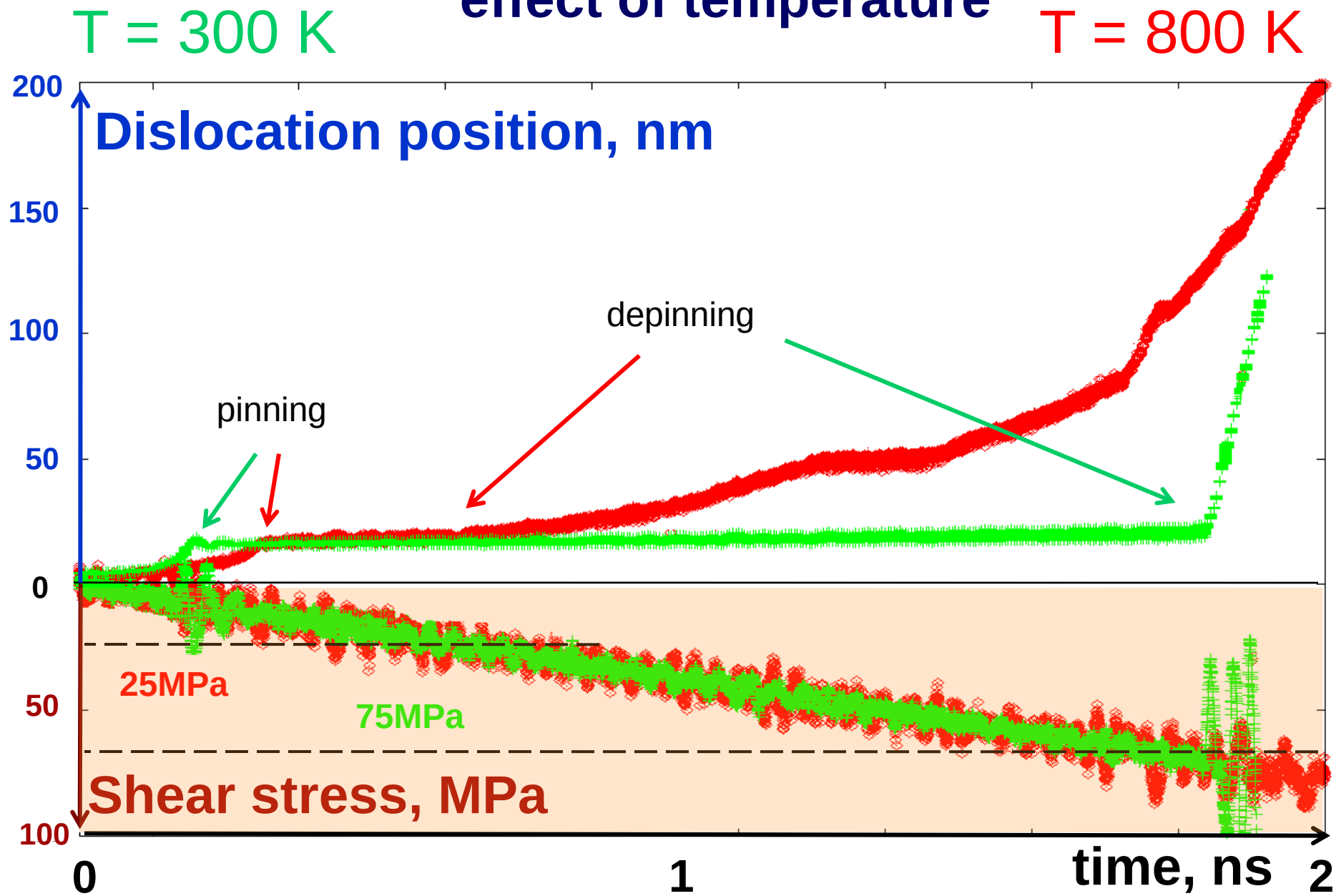


Depinning mechanism

Side view



Dislocation pinning by void: effect of temperature

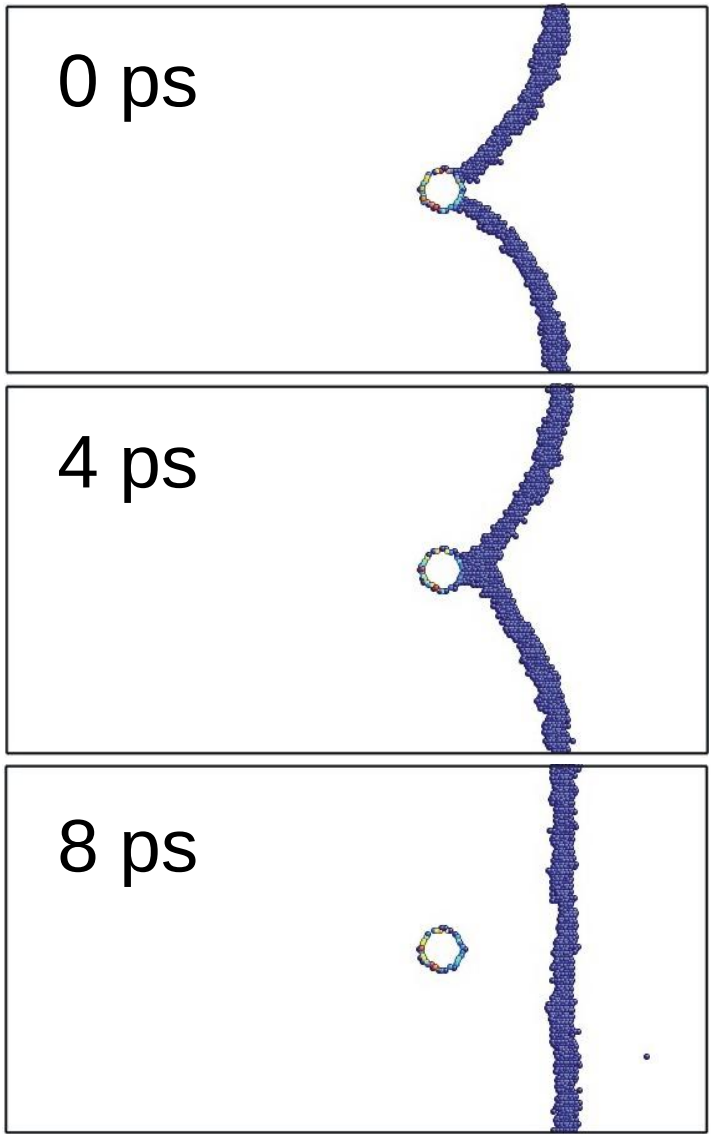


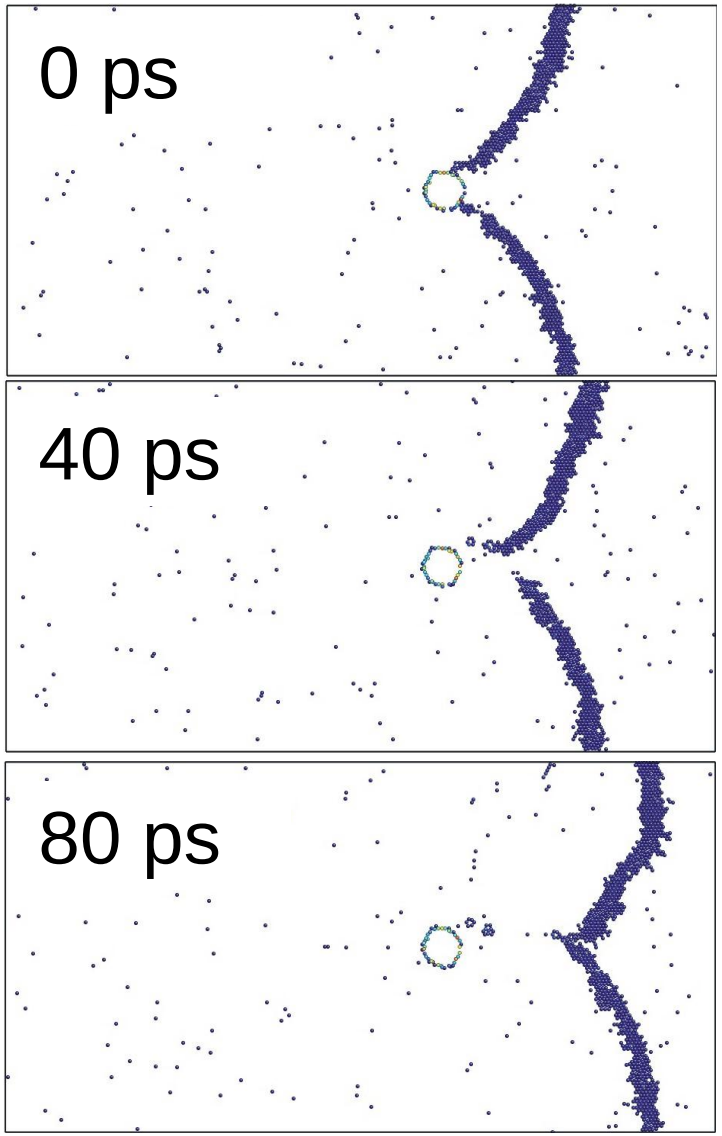
Delay increases with temperature

T = 300 K

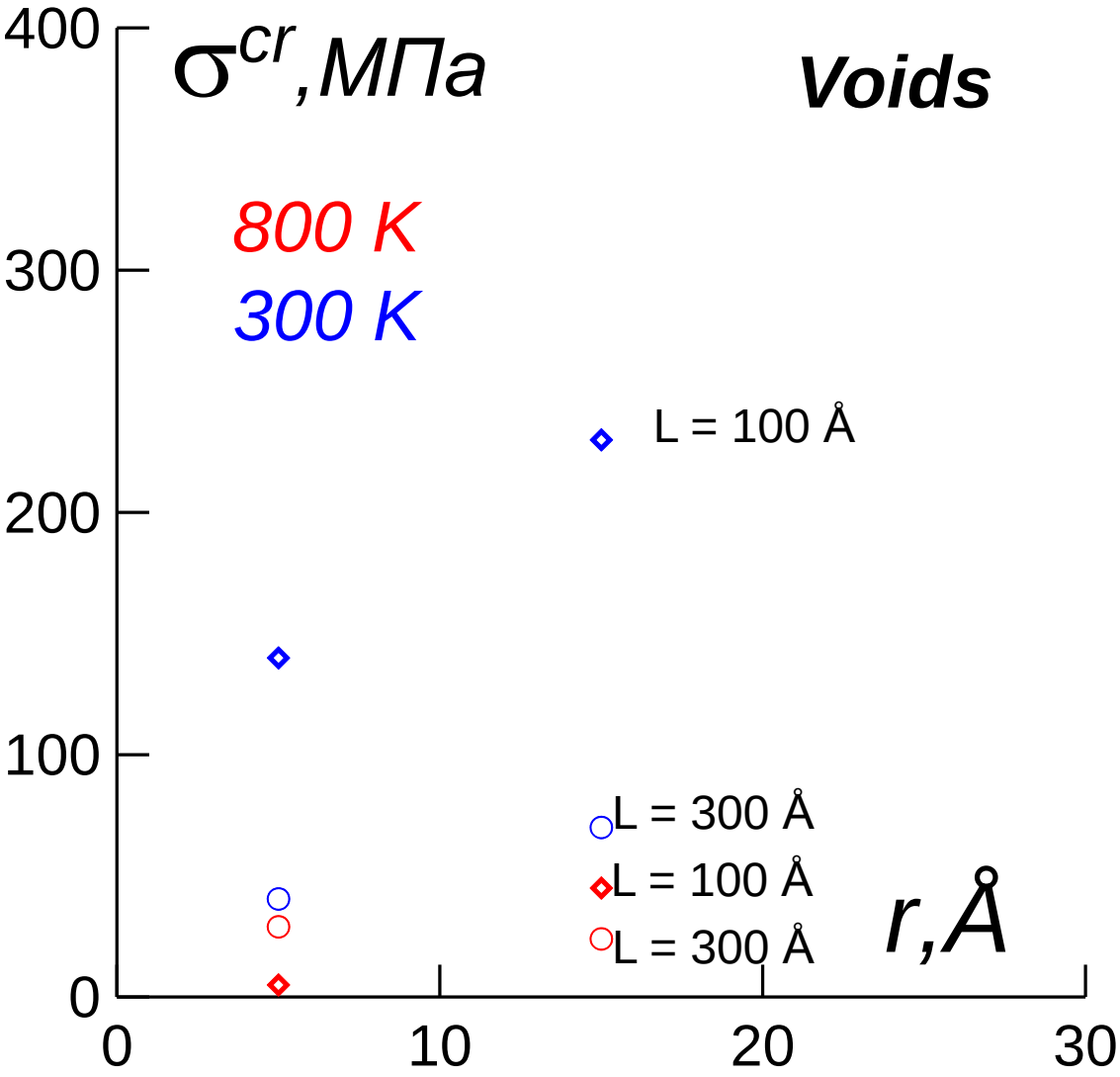
View from above

T = 500 K





Critical resolved shear stress: influence of temperature



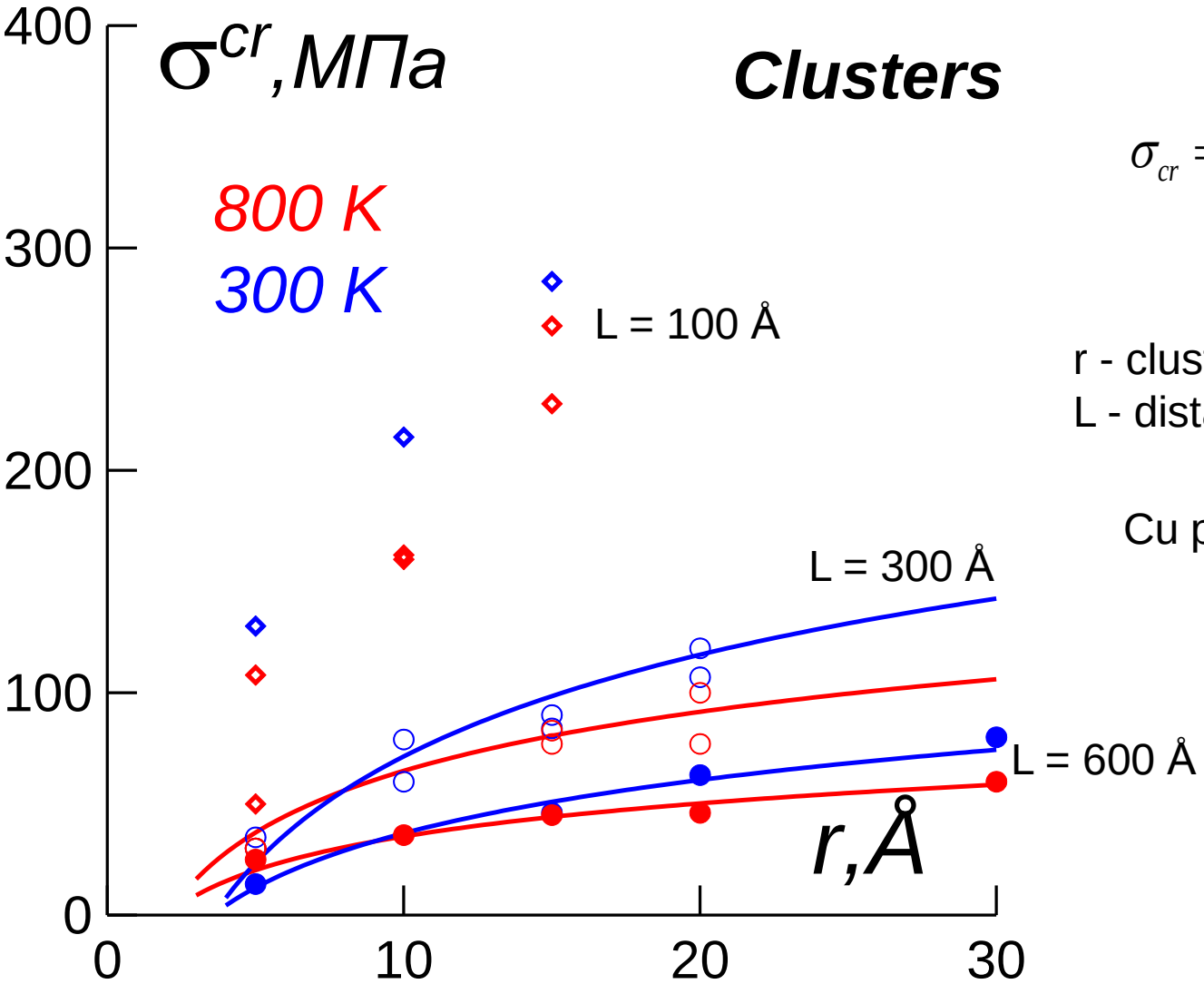
r - void radius
L - distance between voids

Voids in Al

285x220x600 Å
N = 2.1×10^6

285x220x300 Å
N = 1.1×10^6

Critical resolved shear stress: influence of temperature



$$\sigma_{cr} = \frac{A}{L}\log\left[\frac{2r}{B}\cdot\frac{1}{1+\frac{2r}{L}}\right]$$

r - cluster size
L - distance between clusters

Cu precipitate in Al

285x220x600 Å
N = 2.1x10^6

285x220x300 Å
N = 1.1x10^6

Implementation of MD results in continuum model

Implementation of MD results in continuum model

In collaboration with Mayer, Krasnikov, Chelyabinsk, Russia

$$\frac{dS_{zz}}{dt} = \frac{4}{3}G\frac{\partial u}{\partial z} - 2G\frac{dw_{zz}^{\mathrm{pl}}}{dt}$$

The rate of plastic deformation

$$\frac{dw_{zz}^{\mathrm{pl}}}{dt} = -\frac{1}{\sqrt{6}}\boxed{V}\, b\, \rho_D$$

Dislocation motion

$$\frac{m_0}{\left(1-\boxed{V_D}^2/c_t^2\right)^{3/2}}\frac{d\boxed{V_D}}{dt} = -\frac{3}{4}b\left(S_{zz} \pm \frac{2}{3}Y\right) - \boxed{BV_D}$$

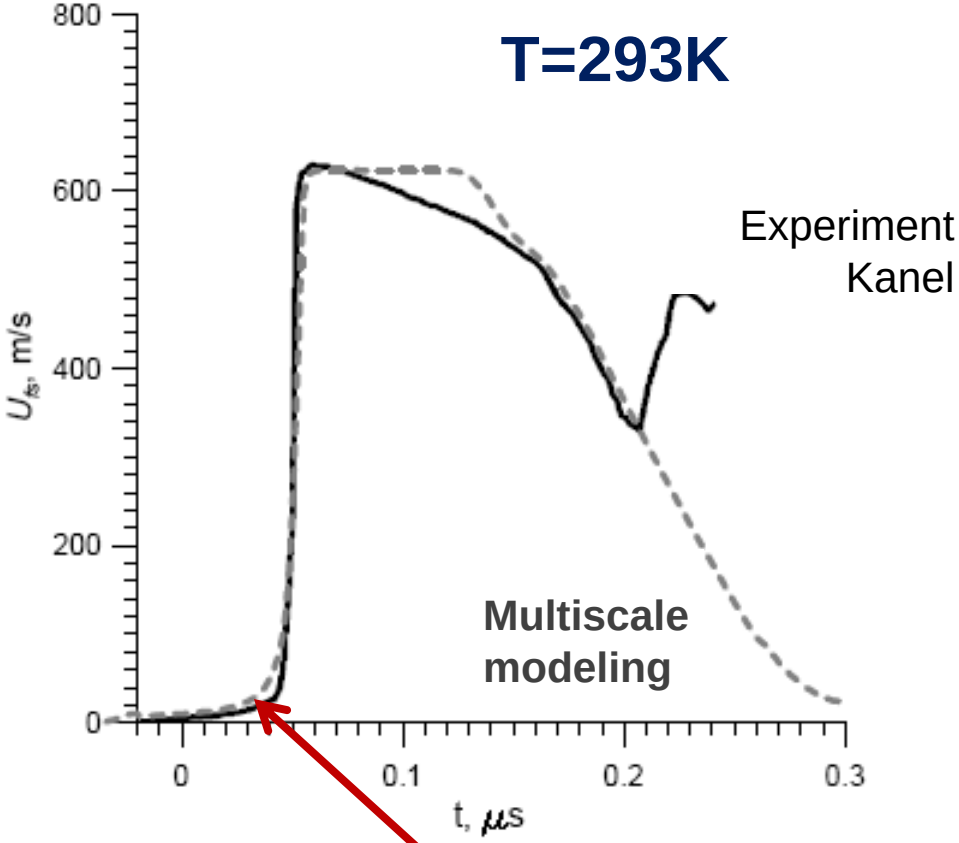
Dislocation density

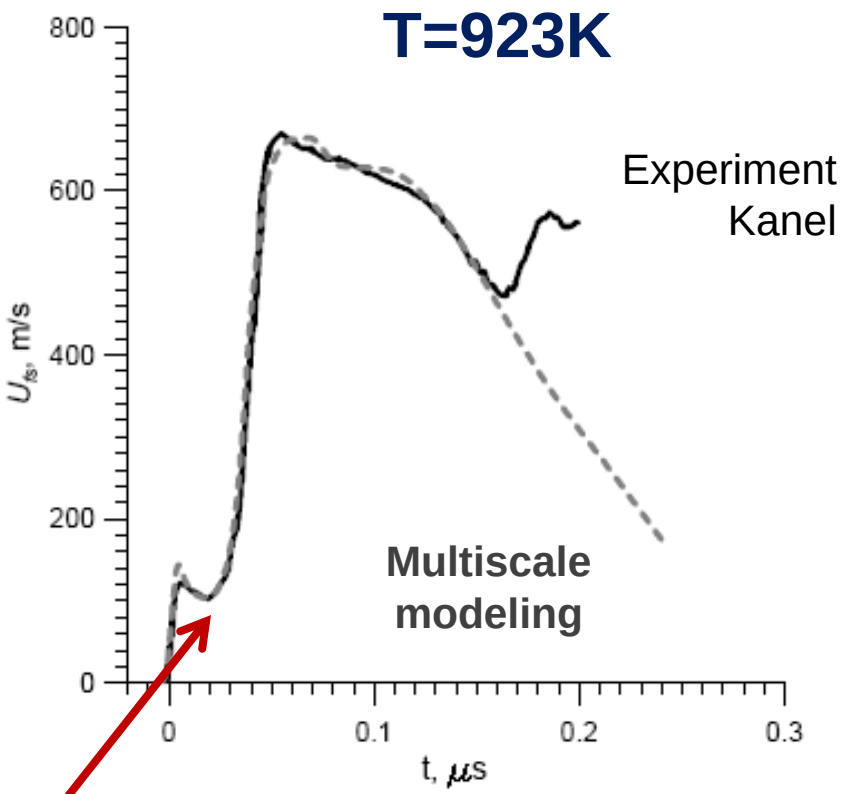
$$\frac{d\rho_D}{dt} = \left(\delta_0\frac{Y_0}{\mu b} + \delta_f\sqrt{\rho_D} - k_a b\cdot\rho_D\right)\cdot\boxed{\left|V_D\right|}\cdot\rho_D$$

Hardening

$$Y = Y_0 + \alpha\mu b\sqrt{\rho_D}$$

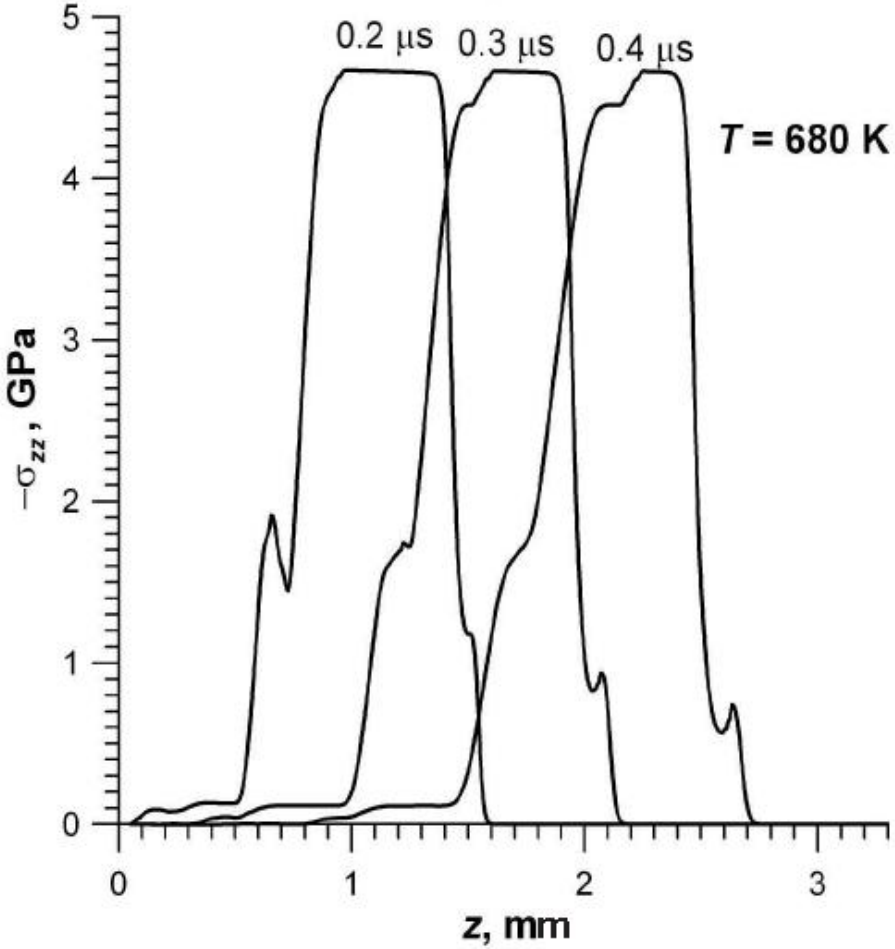
Comparison with shock-wave profiles

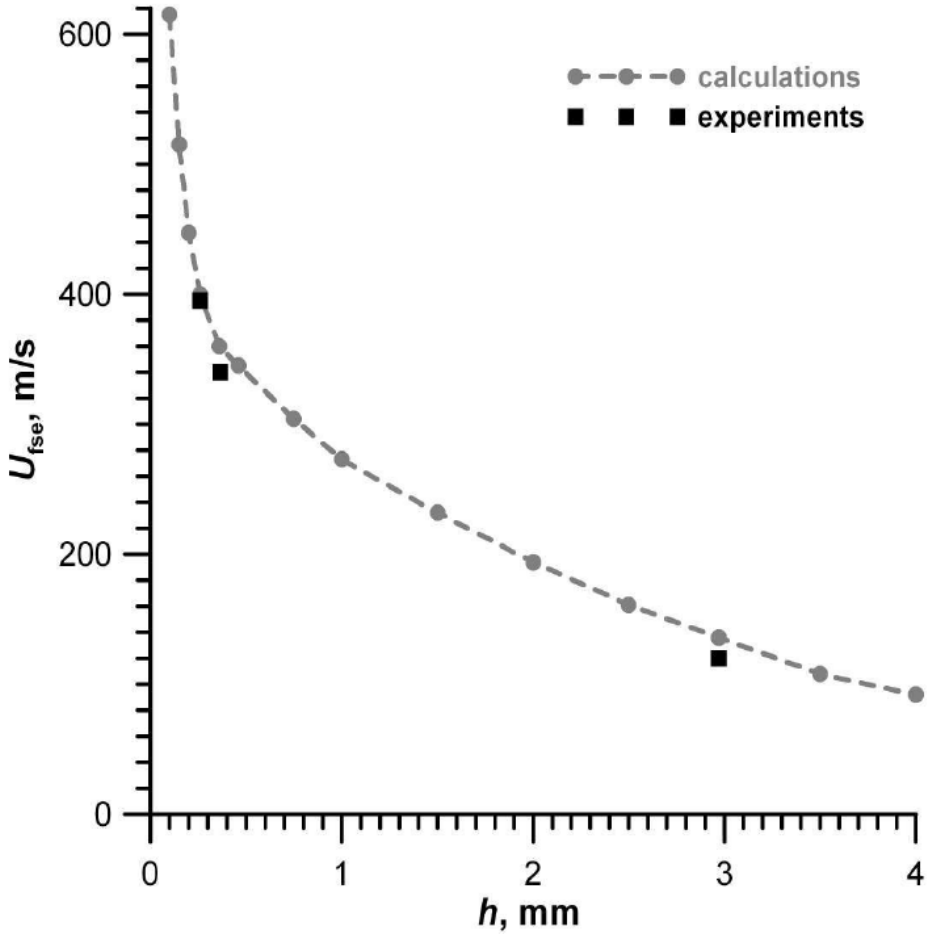




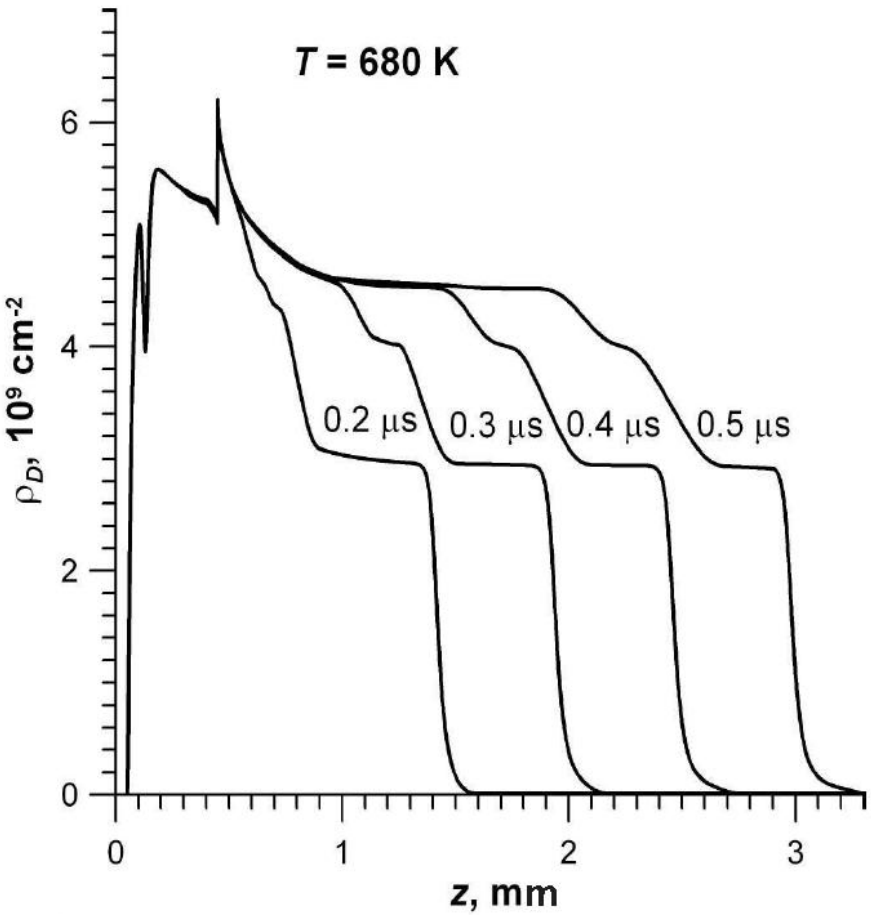
elastic precuror

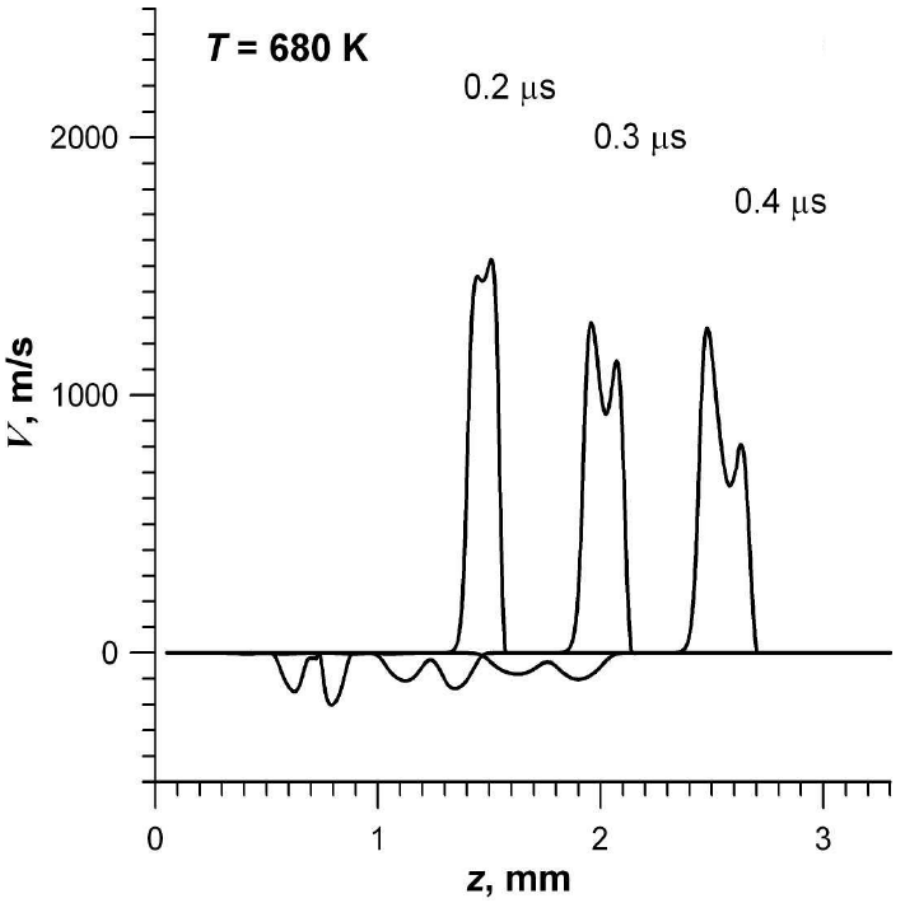
Decreasing of elastic precursor with distance





Microstructure evolution

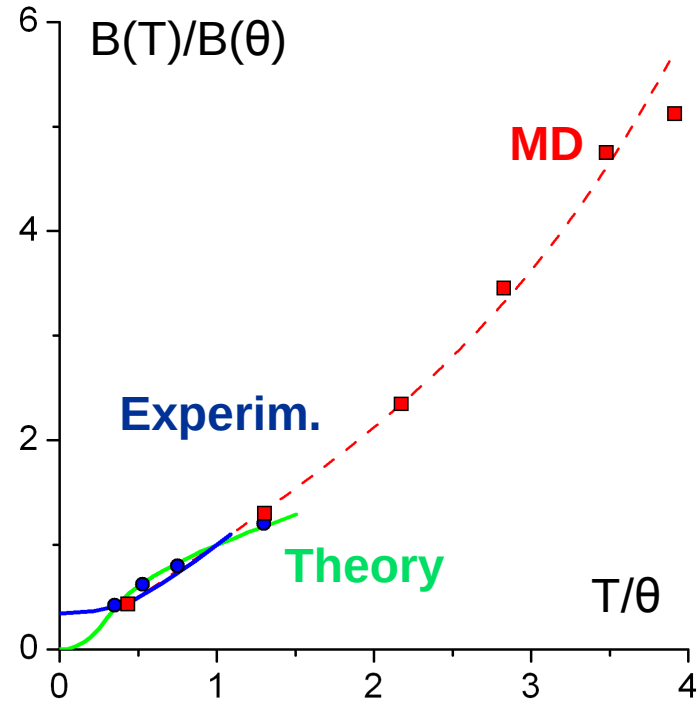
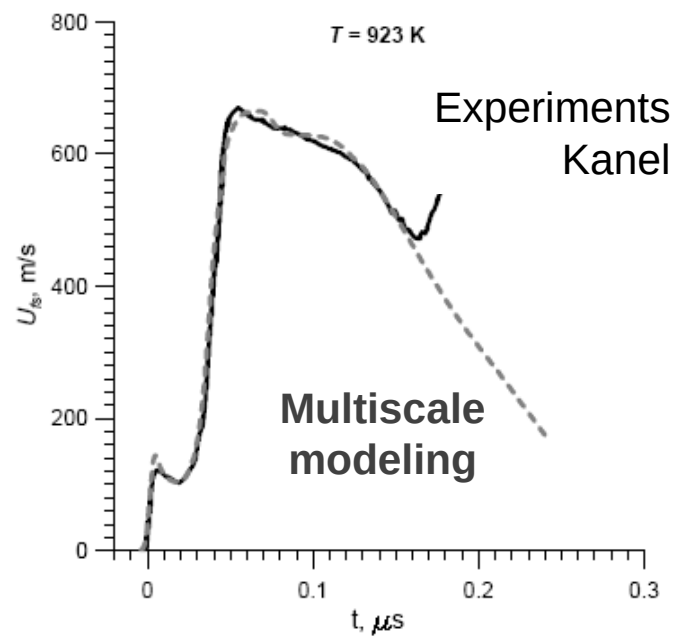




Conclusions

The mechanism of homogeneous nucleation of dislocations is considered.
Nucleation rate of dislocation loops is obtained.

The dependence of phonon drag coefficient B(T)/B(θ) is calculated. Based on MD results dynamic yield stress is estimated.

Different mechanisms of dislocation depinning at different temperatures are observed.

Implementation of MD results in continuum model is proposed. The good agreement of the results of proposed approach with experimental data is obtained.