ПРЕДПРИЯТИЕ ГОСКОРПОРАЦИИ "РОСАТОМ"
ФГУП "ВСЕРОССИЙСКИЙ НАУЧНО-ИССЛЕДОВАТЕЛЬСКИЙ ИНСТИТУТ АВТОМАТИКИ им. Н.Л.Духова"
ЦЕНТР ФУНДАМЕНТАЛЬНЫХ И ПРИКЛАДНЫХ ИССЛЕДОВАНИЙ

# ИСПОЛЬЗОВАНИЕ МНОГОМАСШТАБНОГО ПОДХОДА ДЛЯ ИССЛЕДОВАНИЯ ПЛАСТИЧЕСКИХ СВОЙСТВ МАТЕРИАЛОВ

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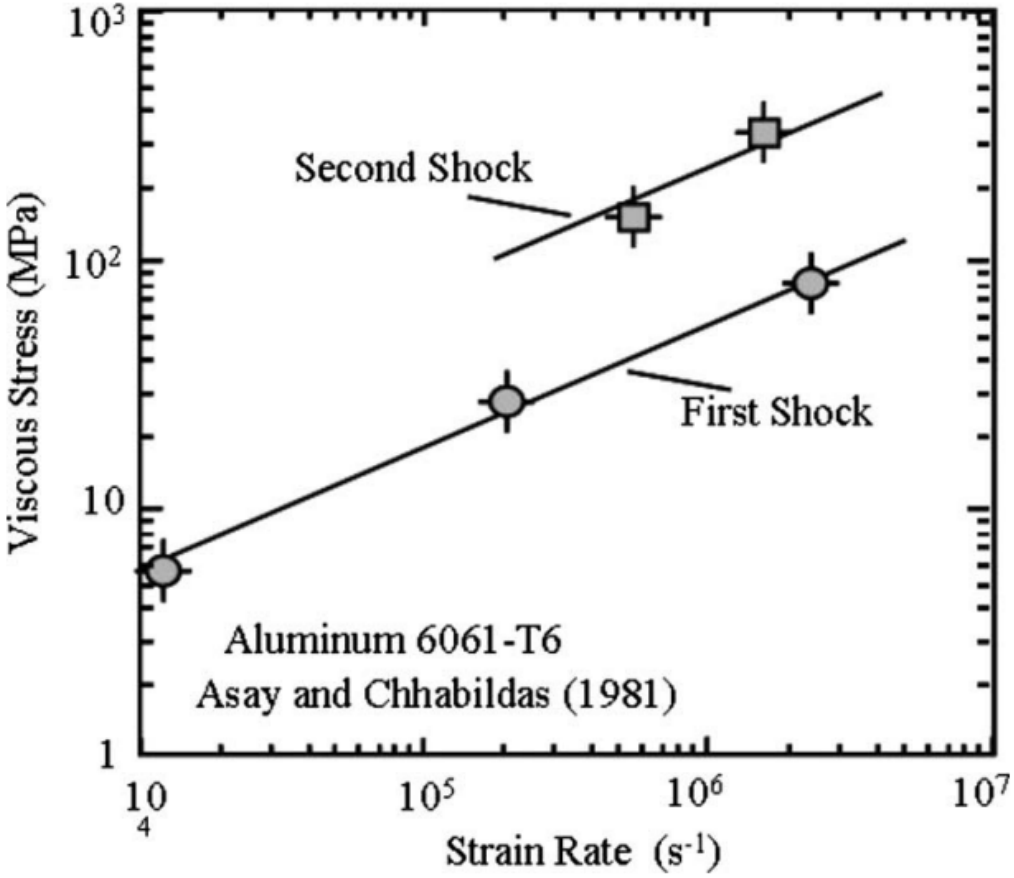
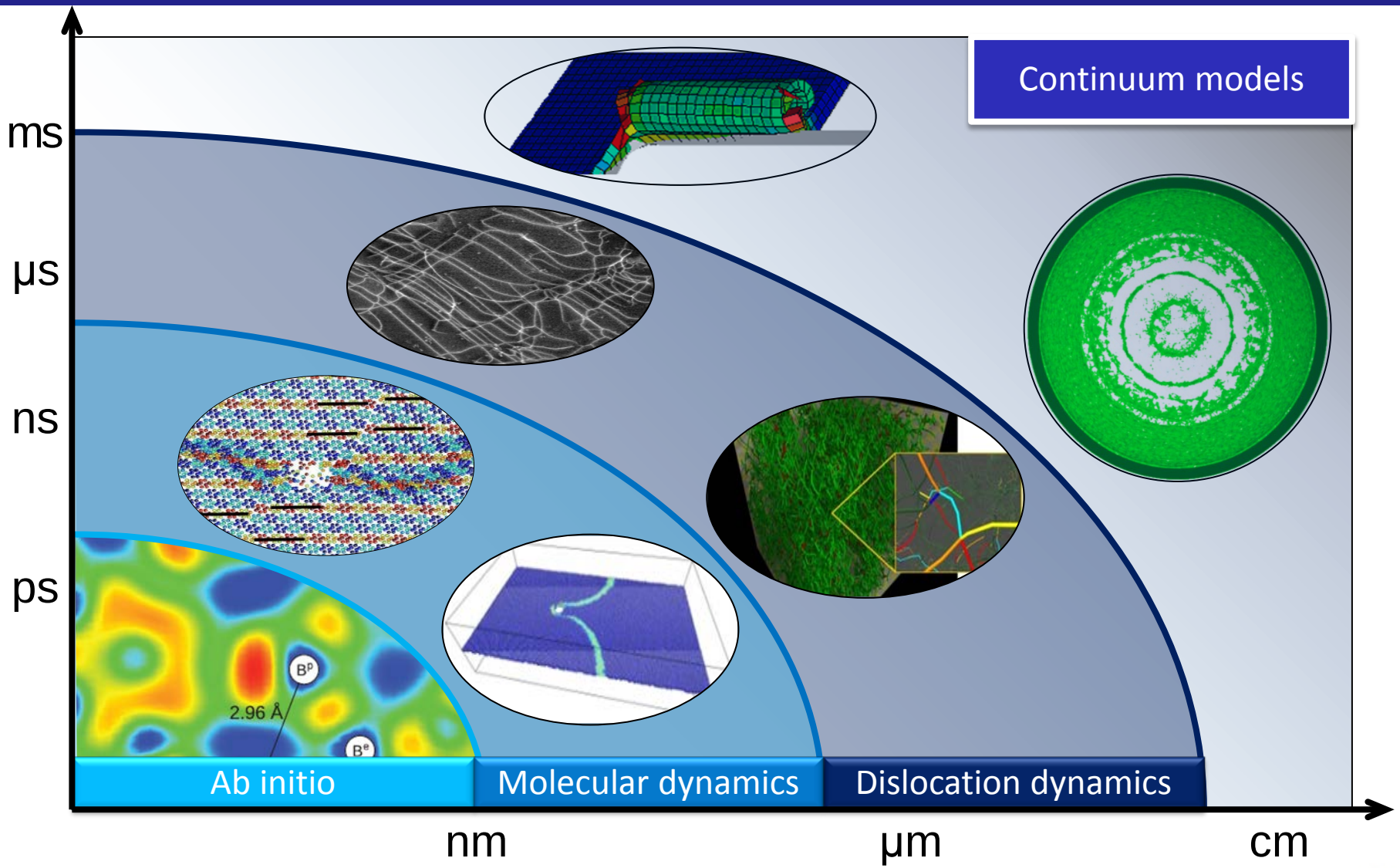
# Crystal plasticity and dislocation density



# Multiscale Materials Modeling



# Plastic response

Twinning

Dislocations

Phase transitions

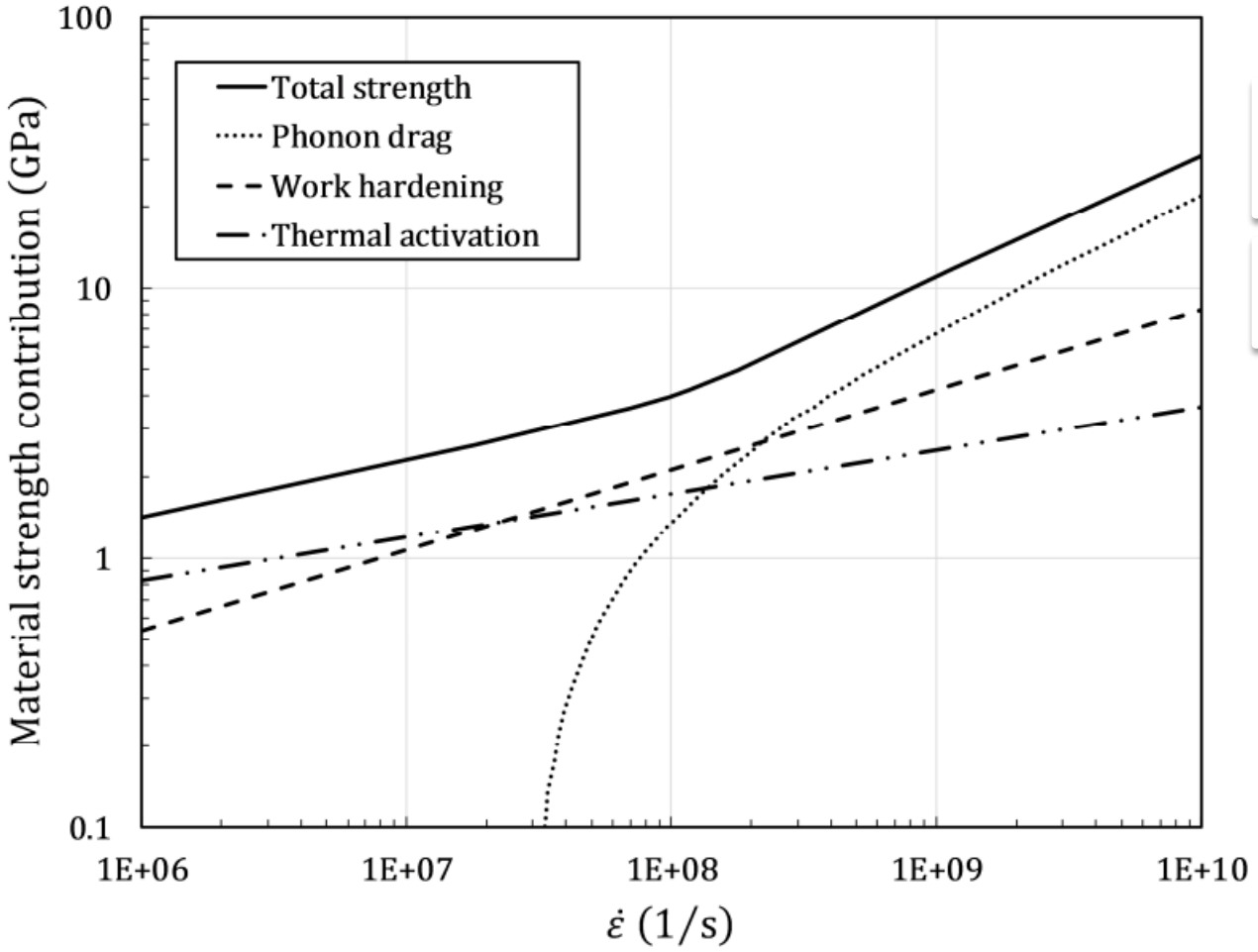
Dislocation mobility

Dislocation density

Dislocation interaction with
- **Other dislocations**
- Voids
- Point defects
- Precipitates

**Large-scale**
Molecular dynamics
Simulations

# Coupling with Dislocation Dynamics

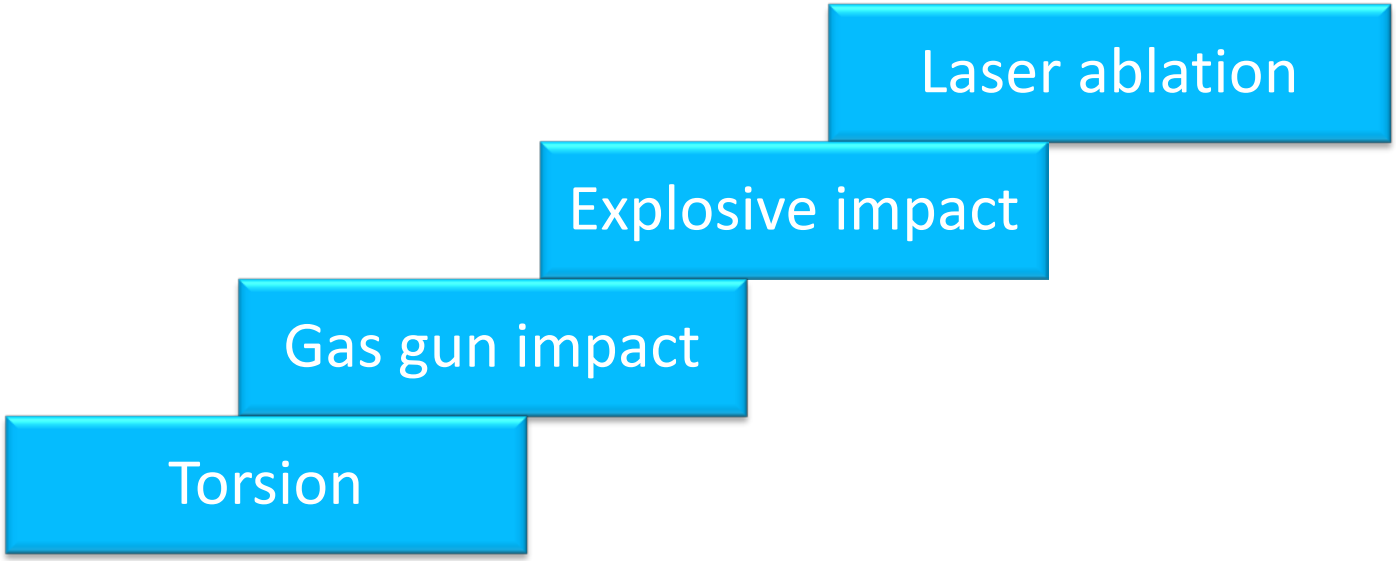


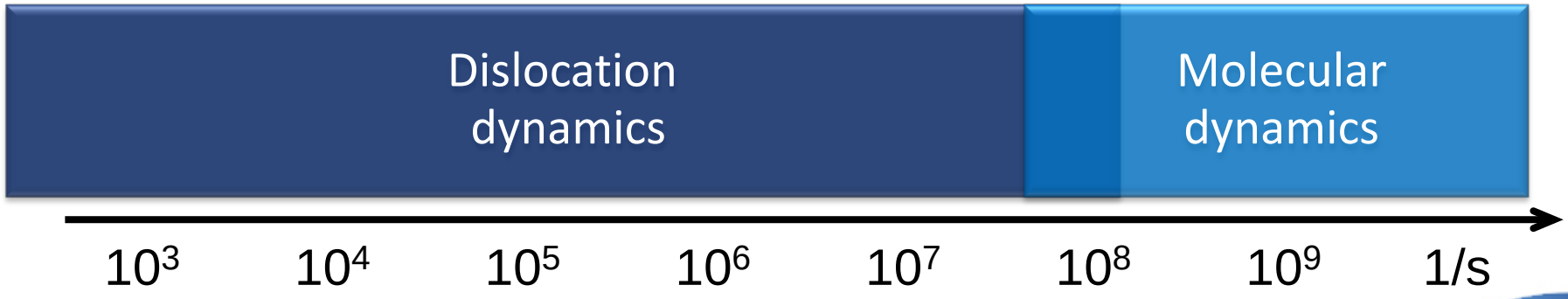

Ta (Remington 2012)

Analyze various mechanisms

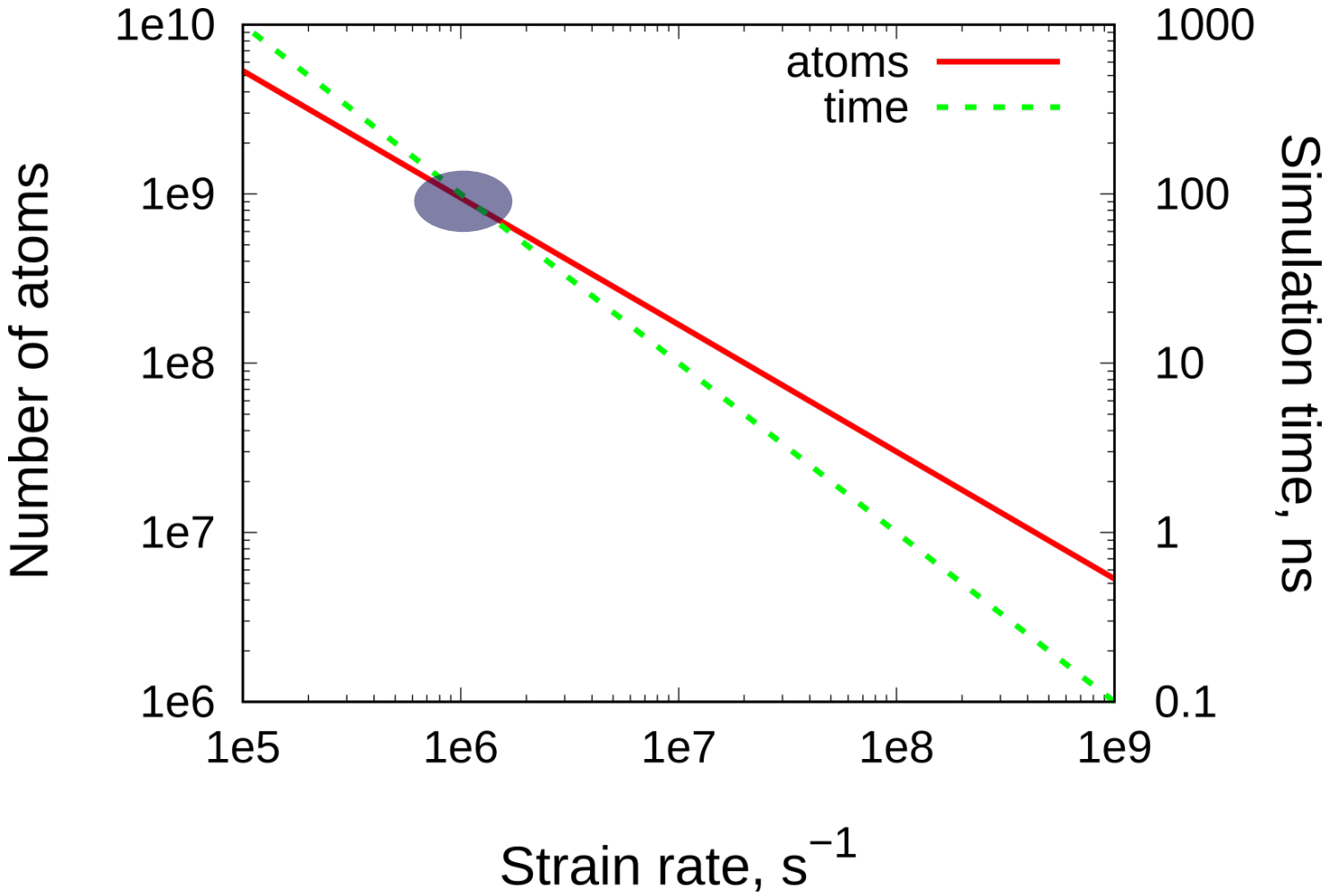
Quantitative prediction

# Strain rate. Experiments and simulations.



# Minimal requirements

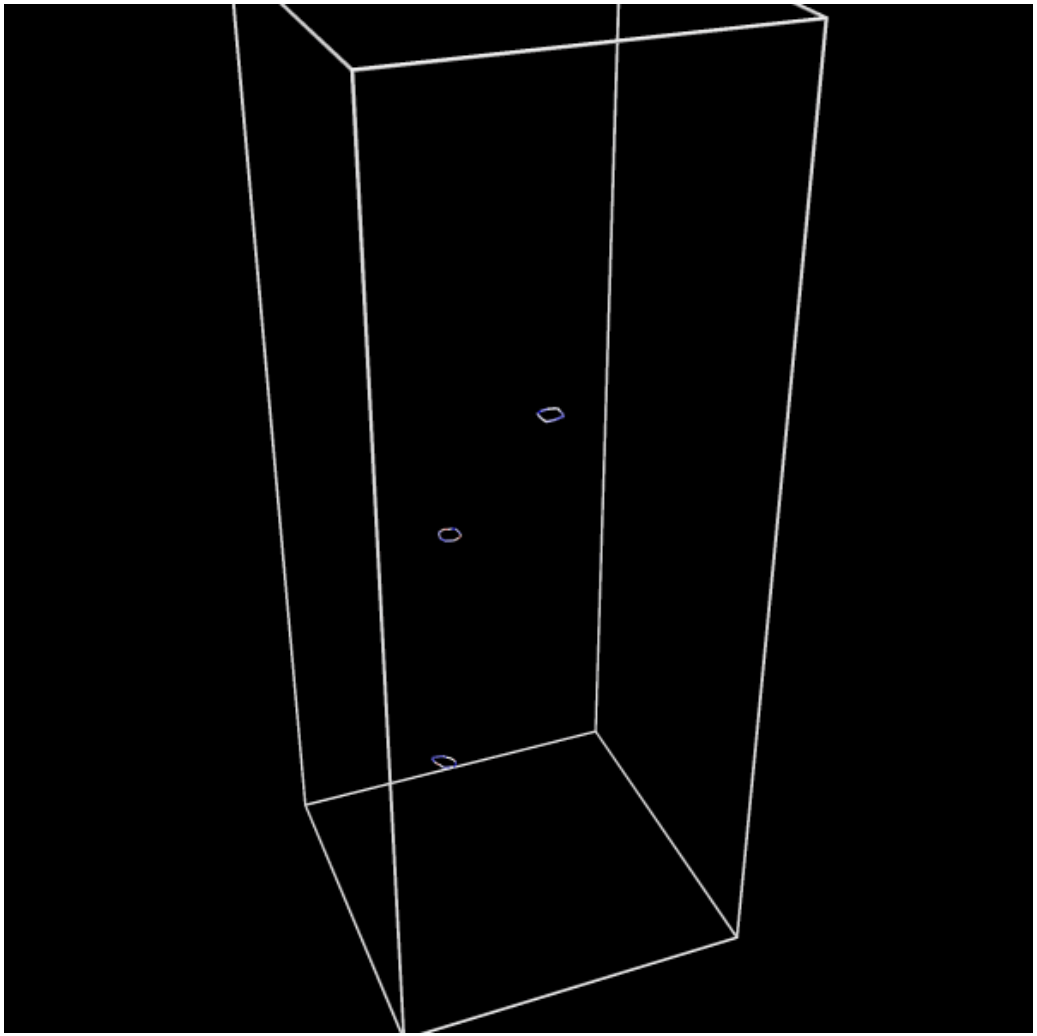



$10^6$/s - maximum

Various temperatures?

# Molybdenum compression

Screw / edge



LAMMPS code - MD

OVITO – visualization

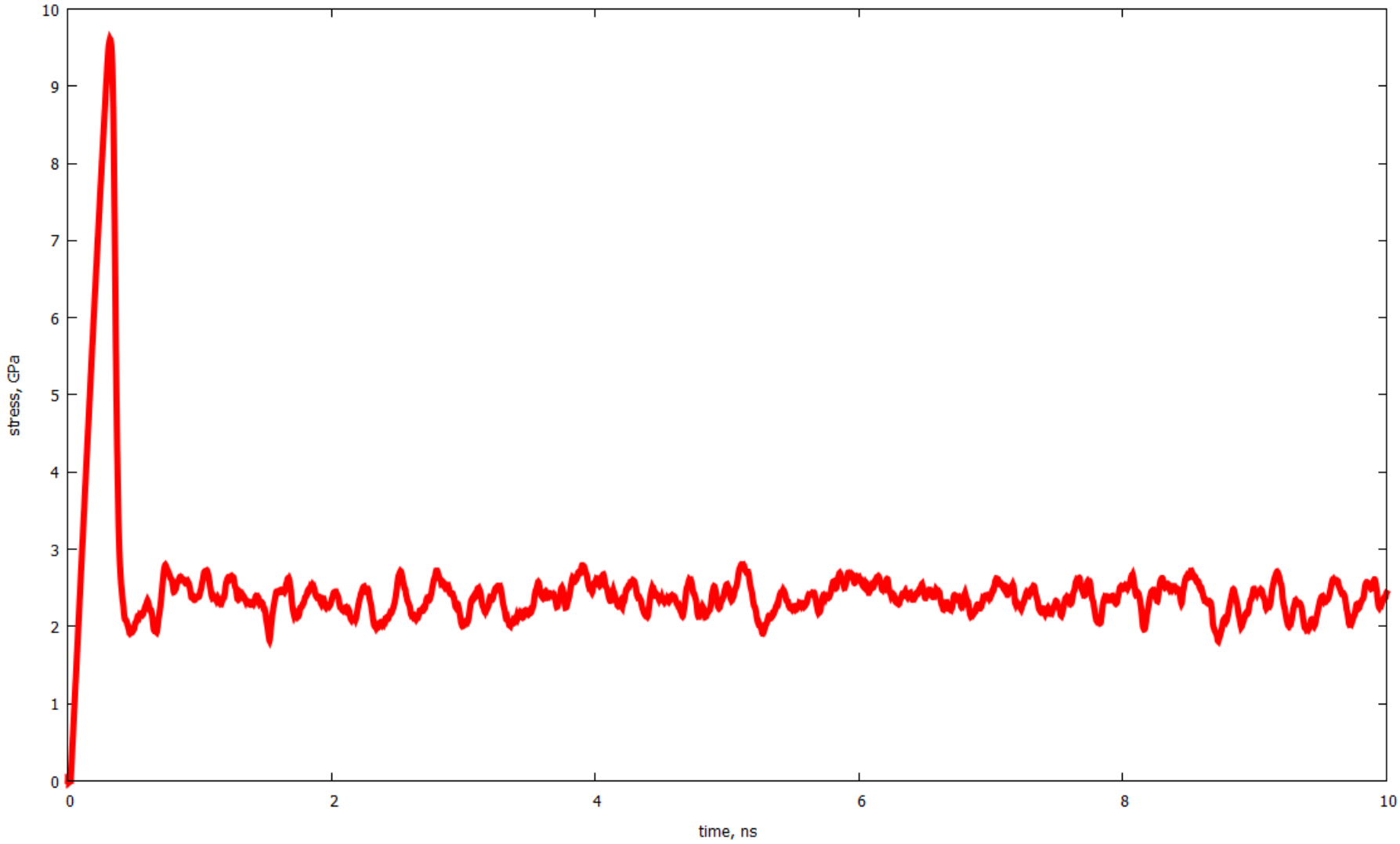
18M Mo atoms

Starikov [2011] - potential

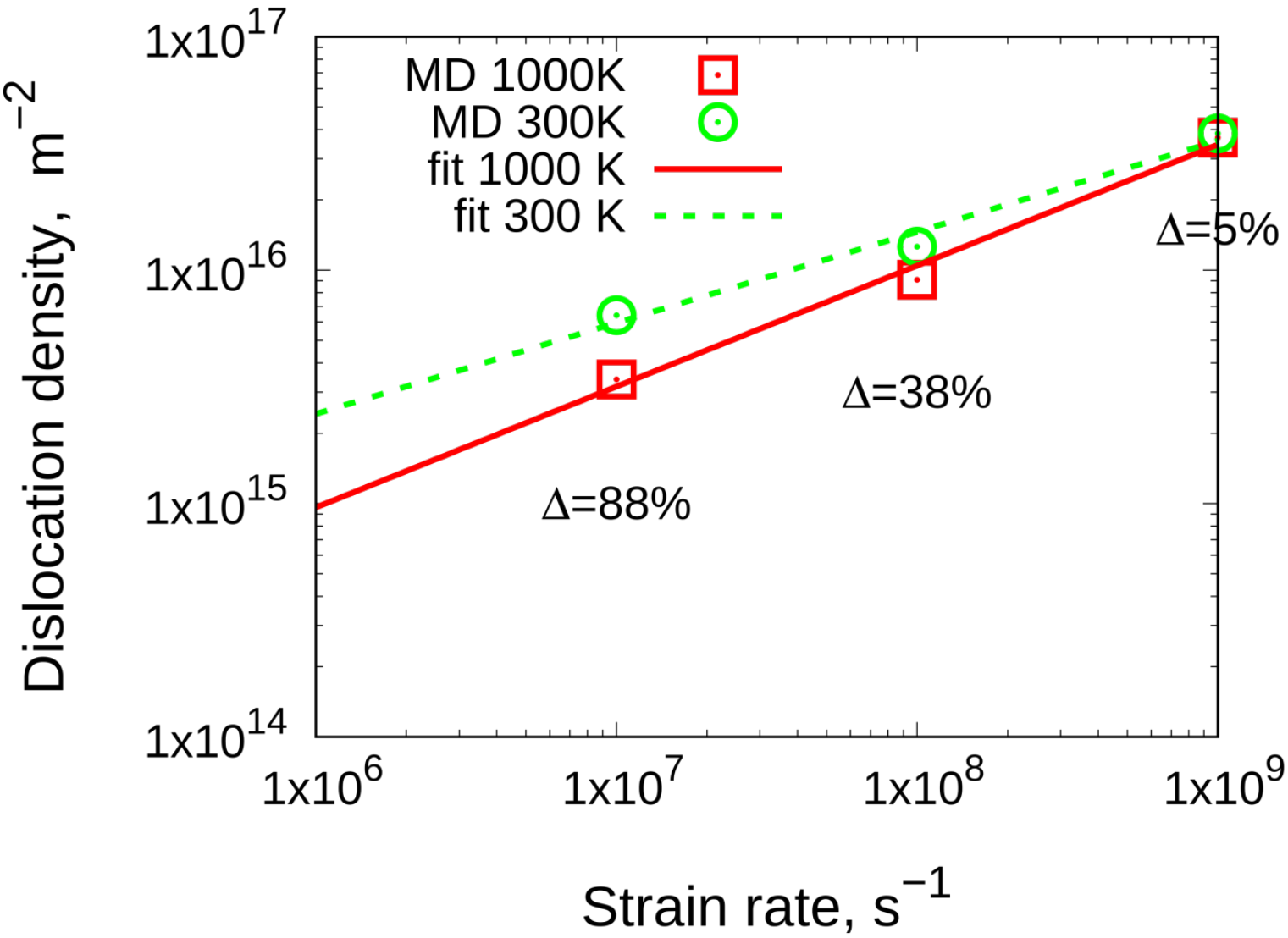
NVT (1000 K)

Const true strain rate $10^8$/s

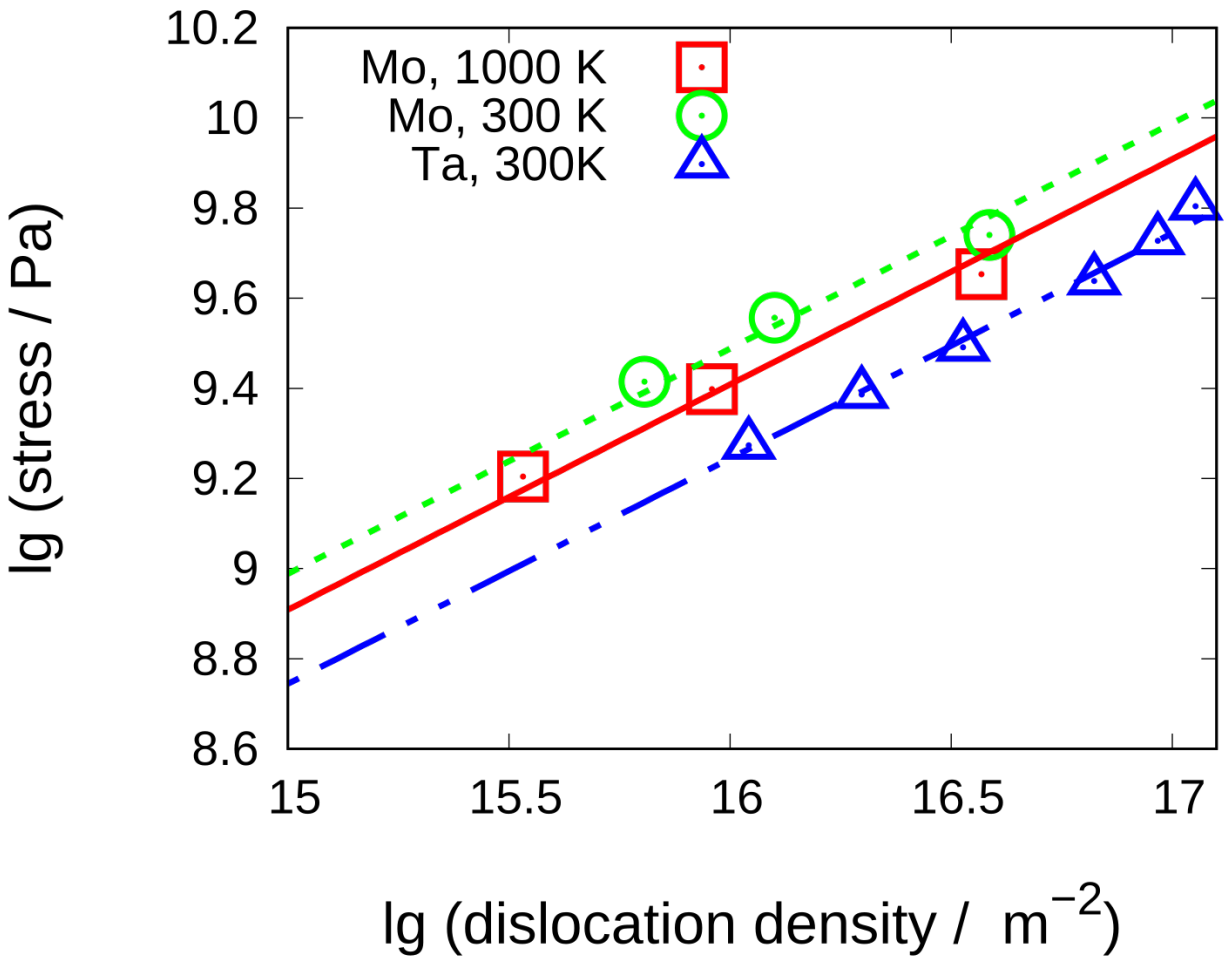
# Stress



# Dislocation density

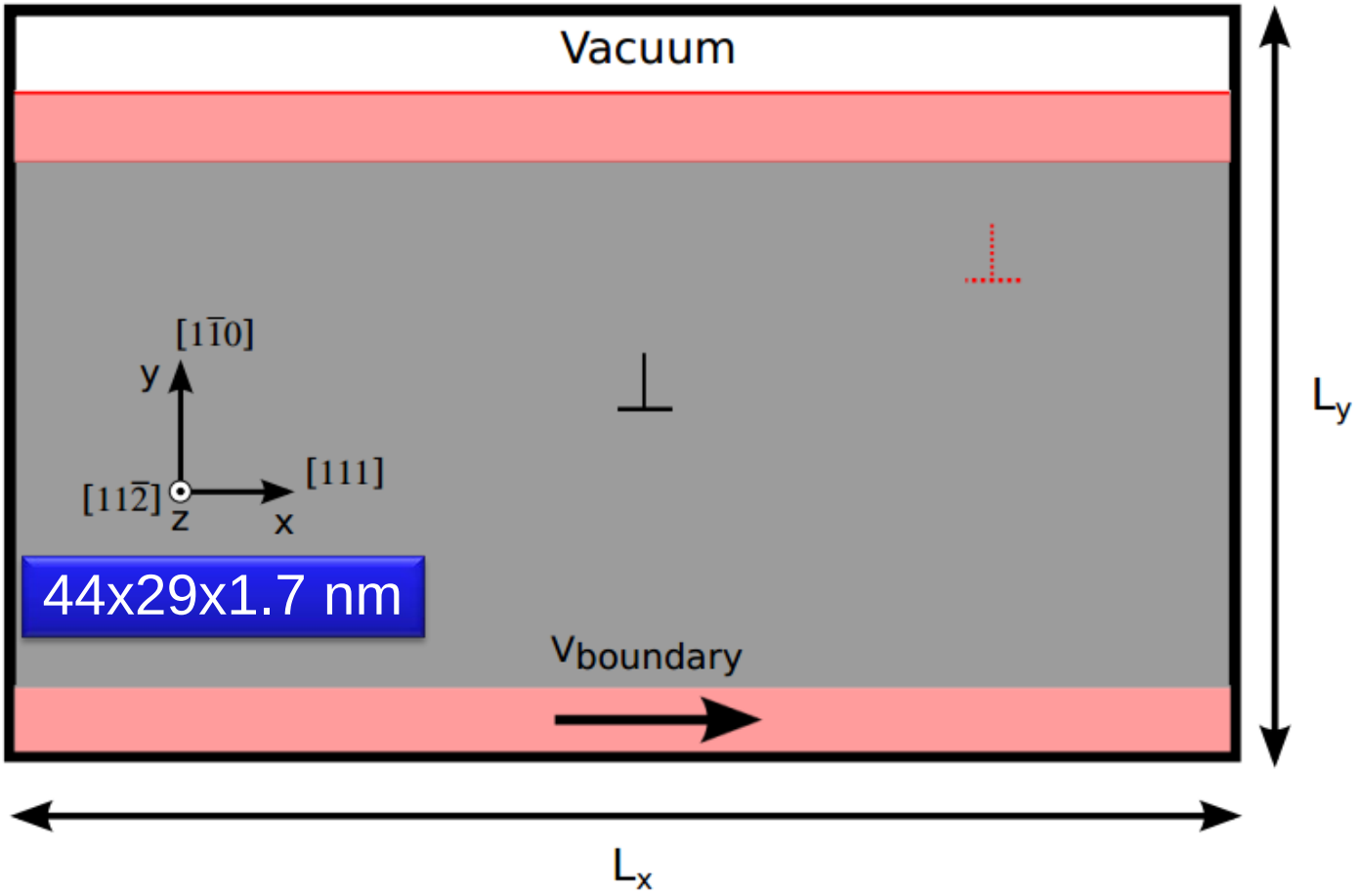


# Taylor hardening

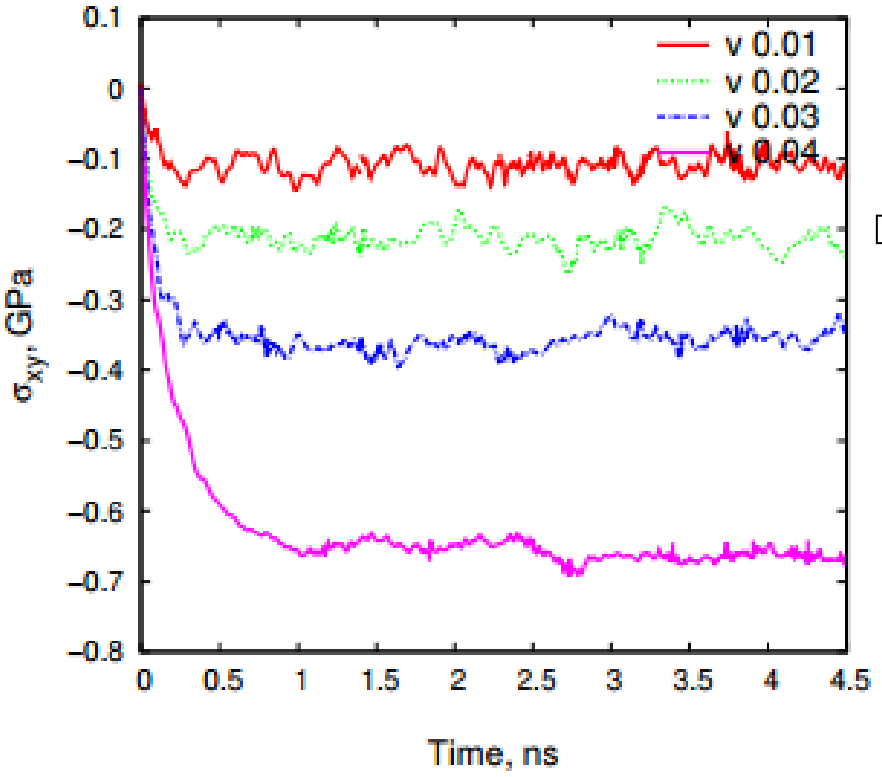



$$\tau = \alpha b G \sqrt{\rho}$$

# Phonon drag. Scheme



# Phonon drag. Results



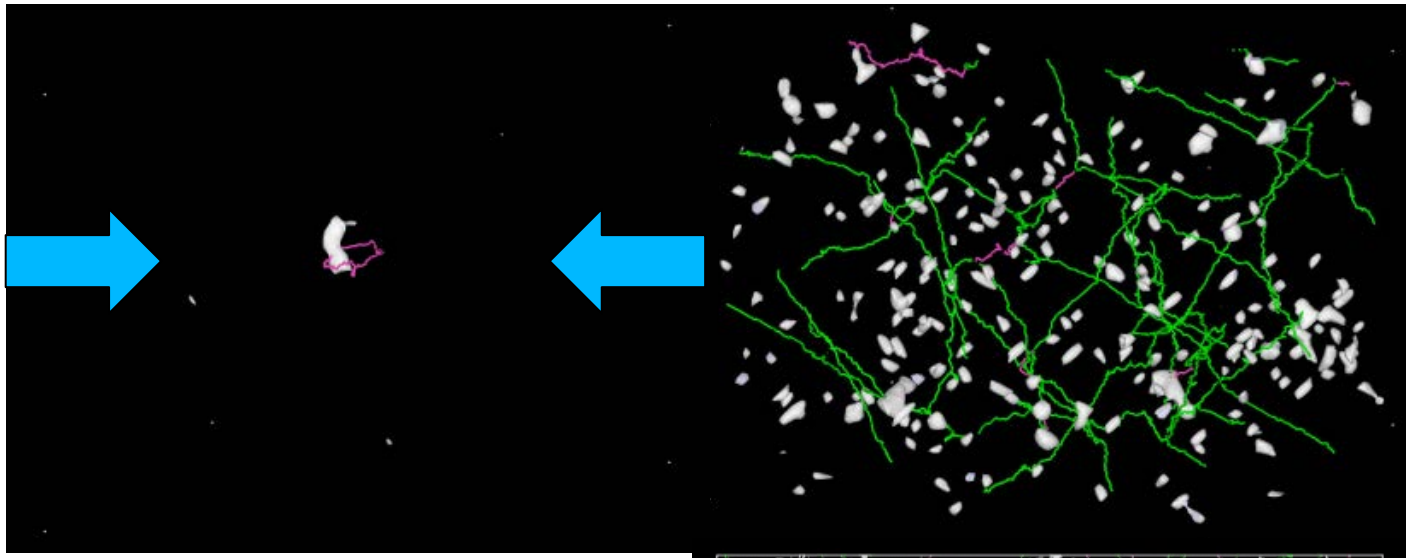

$\sigma(v) \rightarrow B$

- Pressure
- Temperature
- Dislocation density
- Glide velocity

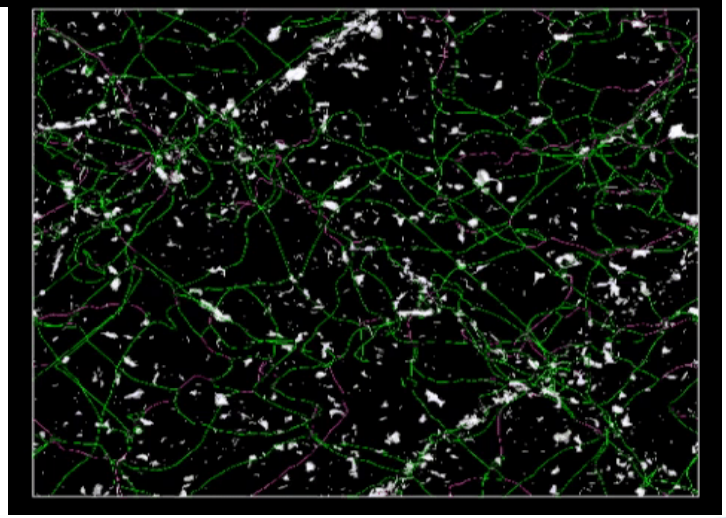
$$v_{disl} = \frac{L_x}{b} v_{bound}$$

$$B = \frac{b\sigma}{v_{disl}}$$

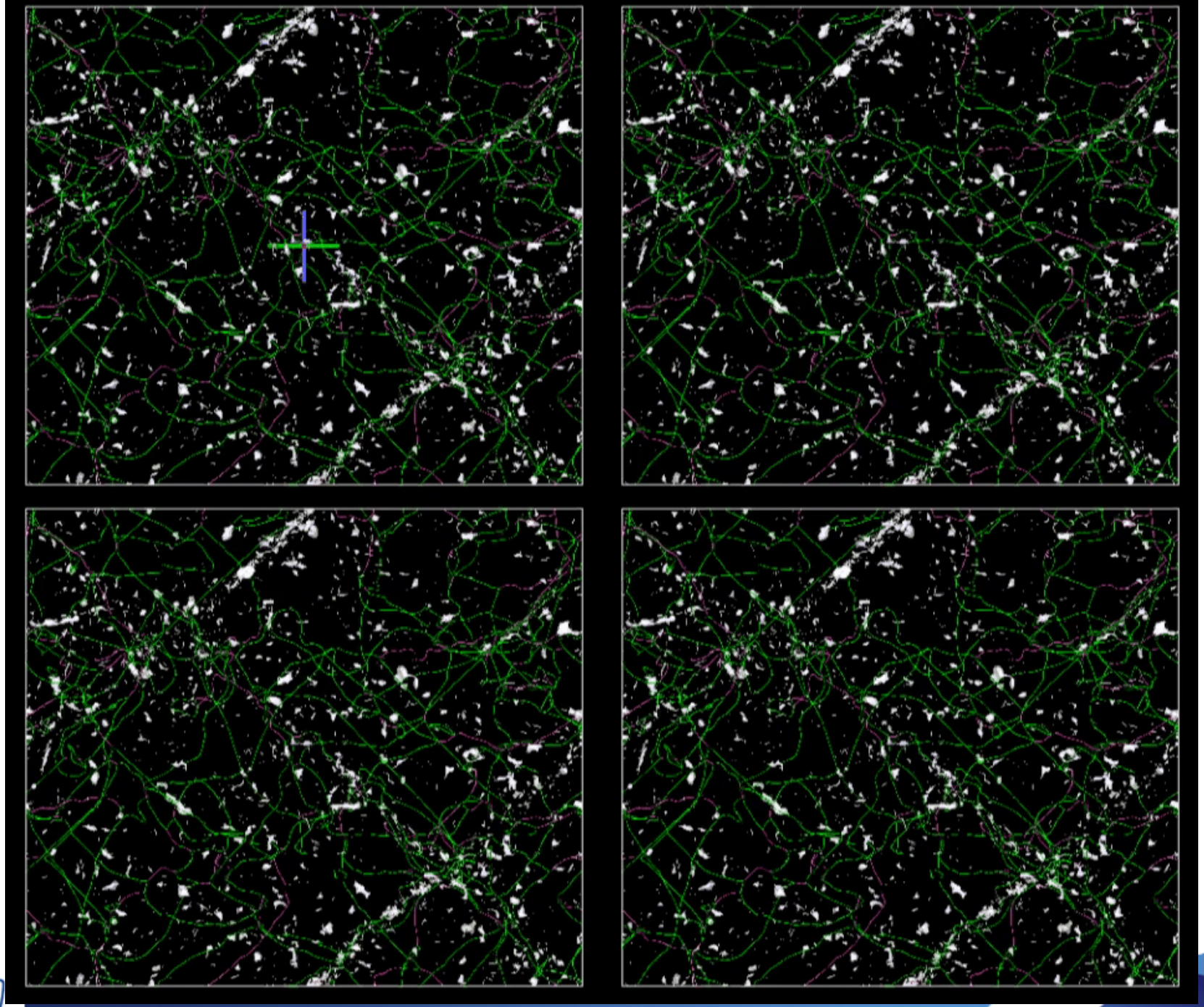
# Molybdenum



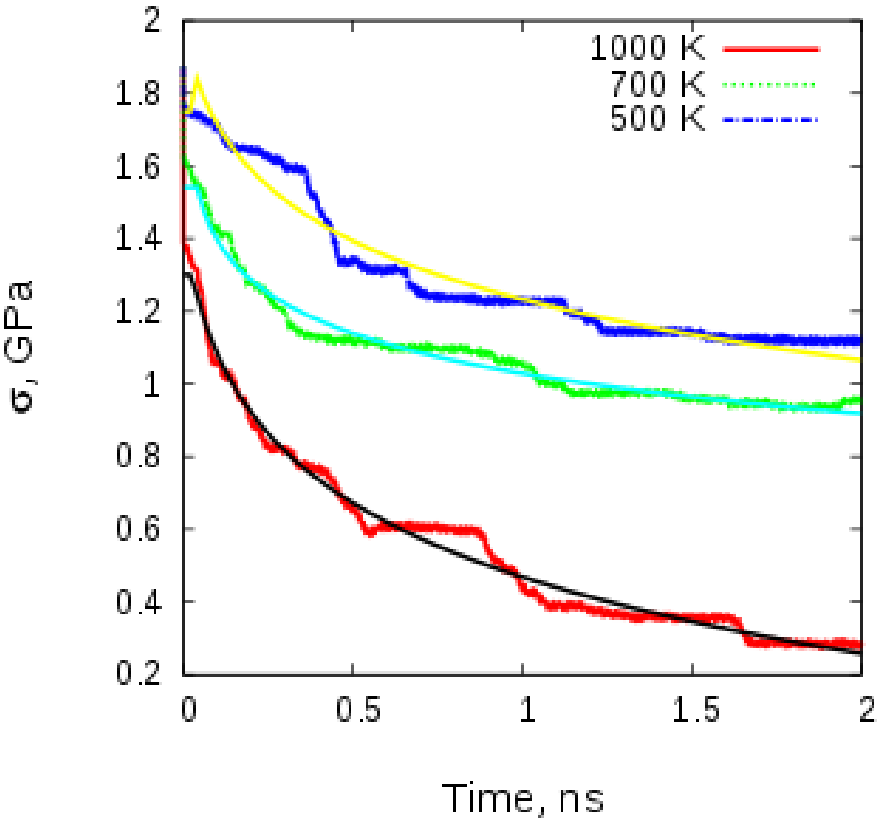
1. Initial dislocation loop
2. Constant strain rate
3. Relaxation
4. Deformation tests

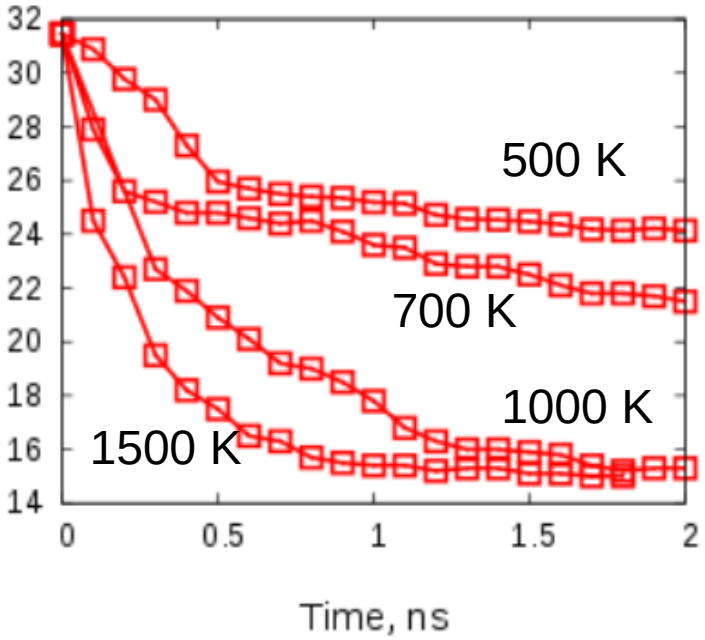


16M atoms



# Relaxation tests

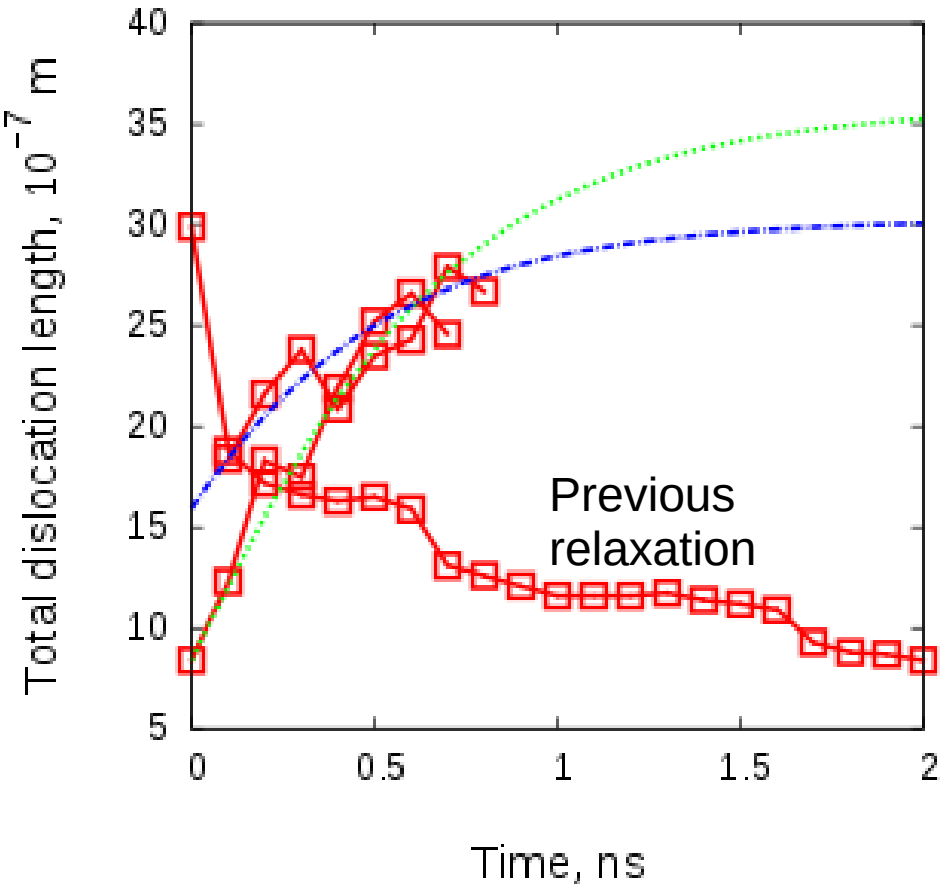



$$\Delta\tau = -\frac{kT}{V_r}\ln(1+\frac{t}{c_r})$$

Activation volume is obtained

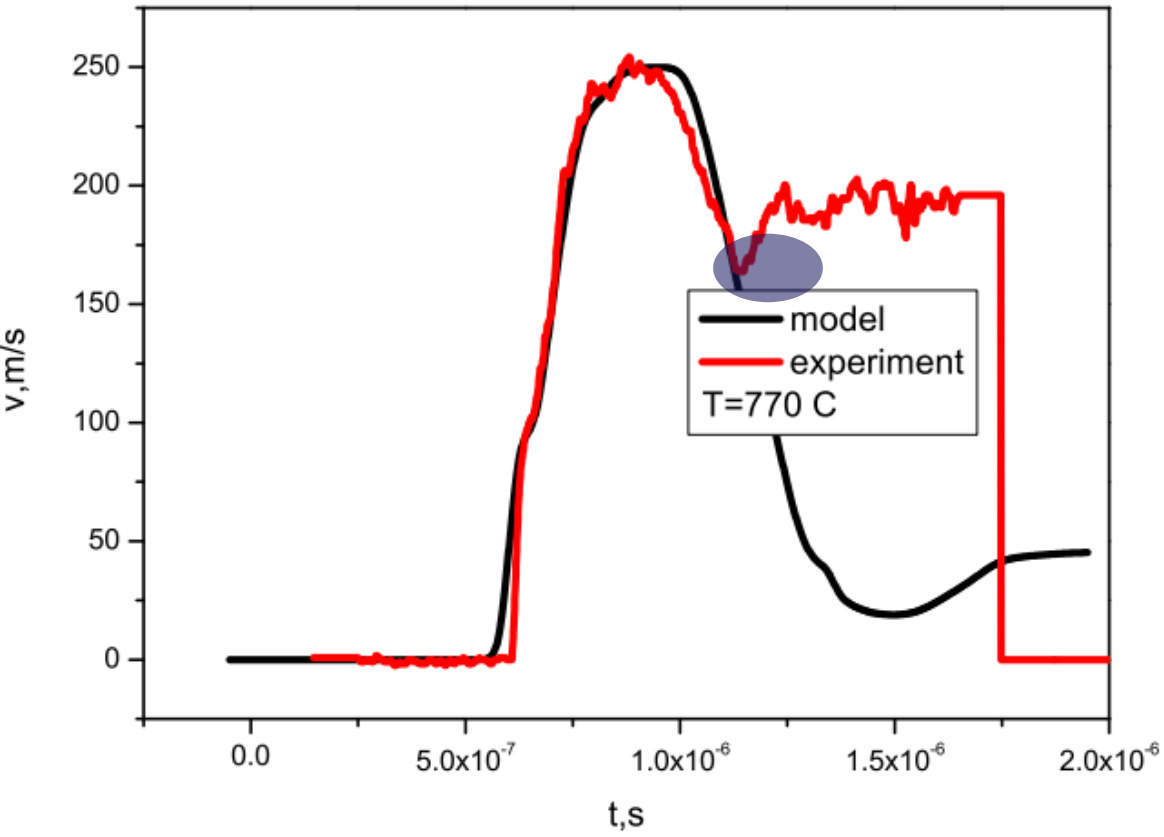
# Repeated deformation




$$\frac{\partial \rho_m}{\partial t} = (\delta_f \sqrt{\rho_m} - k_a b \rho_m) v_d \rho_m$$

Estimation of parameters for dislocation multiplication and annealing

# Coupling with Dislocation Dynamics




No spall model included !

Continuum model

$$\frac{1}{\rho}\frac{d\rho}{dt} = -\frac{\partial u}{\partial z},$$

$$\rho\frac{du}{dt} = \frac{\partial \sigma_{zz}}{\partial z},$$

$$\rho\frac{dE}{dt} = -\frac{\sigma_{zz}}{\rho}\frac{d\rho}{dt} + \frac{\partial}{\partial z}\left(K\frac{\partial T}{\partial z}\right),$$

$$\sigma_{zz} = -P(\rho, E) + S_{zz},$$

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

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

$$\frac{m_0}{(1-V^2/c_t^2)^{3/2}}\frac{dV}{dt} = -\frac{3}{4}b\left(\sqrt{\frac{2}{3}}S_{zz} \pm \frac{2}{3}Y\right) - B(V, T)V.$$

# Conclusions

- Obtain parameters for DD
- Studying various mechanisms
- New insights

# Thanks

Alexey V. Yanilkin

Denis K. Il’nitsky