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MODELS OF FRACTURE FROM ATOMISTIC SIMULATIONS

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Molecular Dynamics Models

Single crystal metal

EAM potential

$$E = \sum_{i>j} \Phi_{ij}\left(r_{ij}\right) + \sum_{i} F_i\left(\rho_i\right)$$

Simple liquid

Lennard-Jones potential

$$E = \sum_{i>j} 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

$$r_{cut} = 4.0\sigma$$

Aluminum

- X.-Y. Liu, F. Ercolessi, J.B. Adams

MSMSE **12,** 665 (2004)

- X.-Y. Liu, Wei Xu, S.M. Foiles, J.B. Adams APL **72,** 1578 (1998)
- Y.Mishin, D.Farkas, M.J.Mehl,

D.A.Papaconstantopoulos

PRB **59,** 3393 (1999)

Hexane

energy	ε	413 K
distance	σ	5.909 Å
mass	m	$1.4 \cdot 10^{-22}$ g
time	τ	2.96 ps
pressure	ε/σ^3	27.64 MPa

Lennard - Jones (LJ) potential for Hexane

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

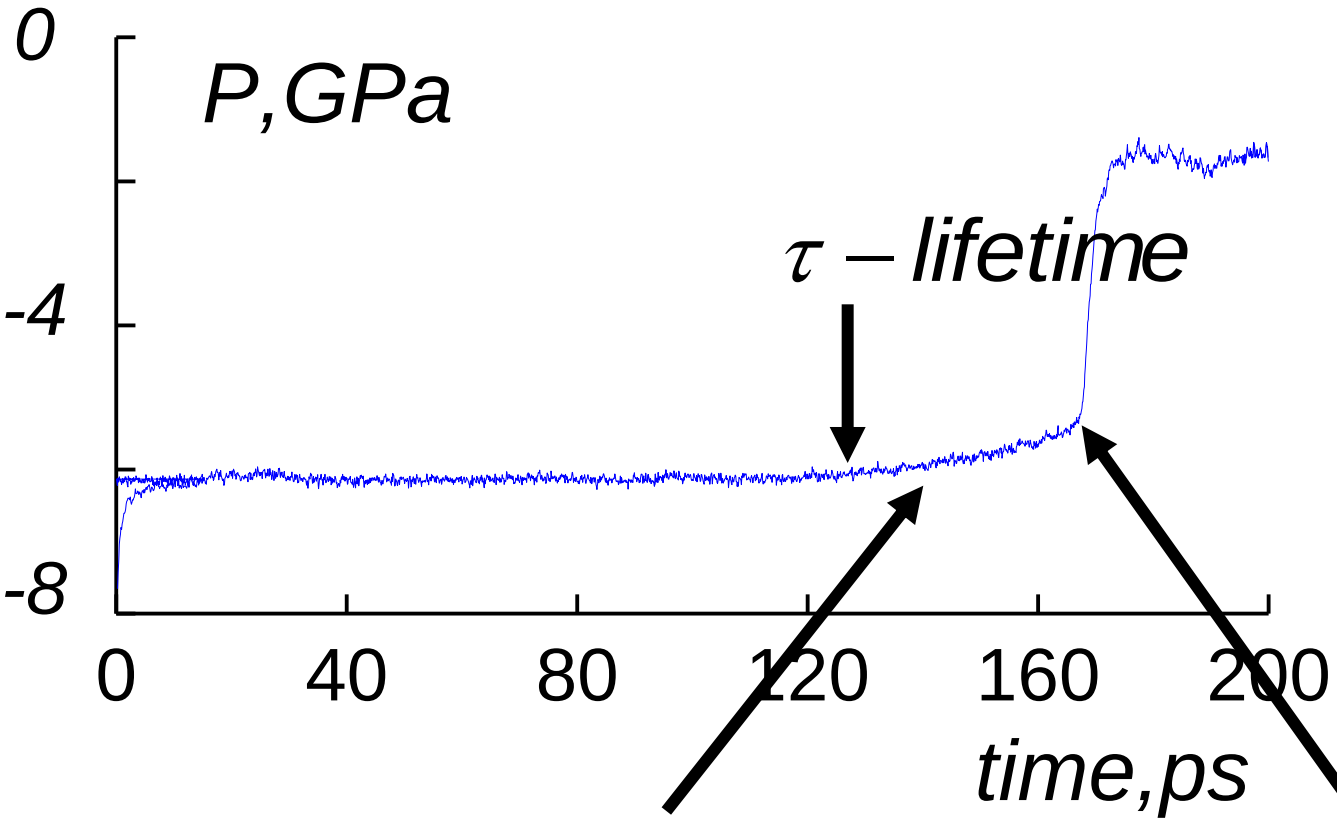
$$r_{cut} = 4.0\sigma$$

energy	ε	413 K
distance	σ	5.909 Å
mass	m	$1.4 \cdot 10^{-22}$ g
time	τ	2.96 ps
pressure	ε/σ^3	27.64 MPa

	Experiment	LJ model
Density	0.66 g/cm^3	0.58 g/cm^3
Viscosity	0.31 cP	0.26 cP
Surf. Tension	18.4 dyne/cm	~16 dyne/cm
Sound speed	1.1 km/s	~0.75 km/s

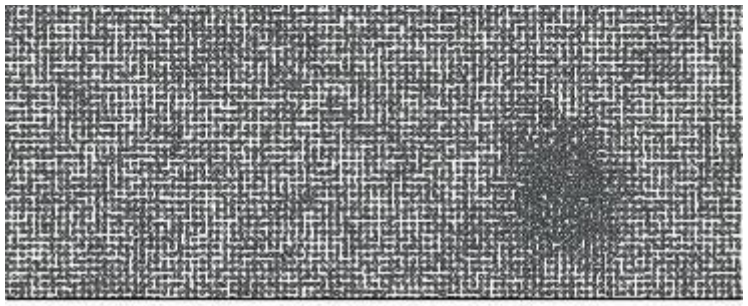
Nucleation rate: single crystal

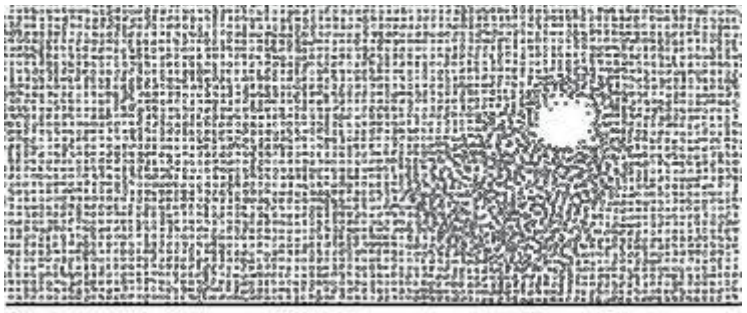
Spontaneous nucleation of voids



Al, T = 700 K

$$J = \frac{1}{\langle \tau \rangle N}$$

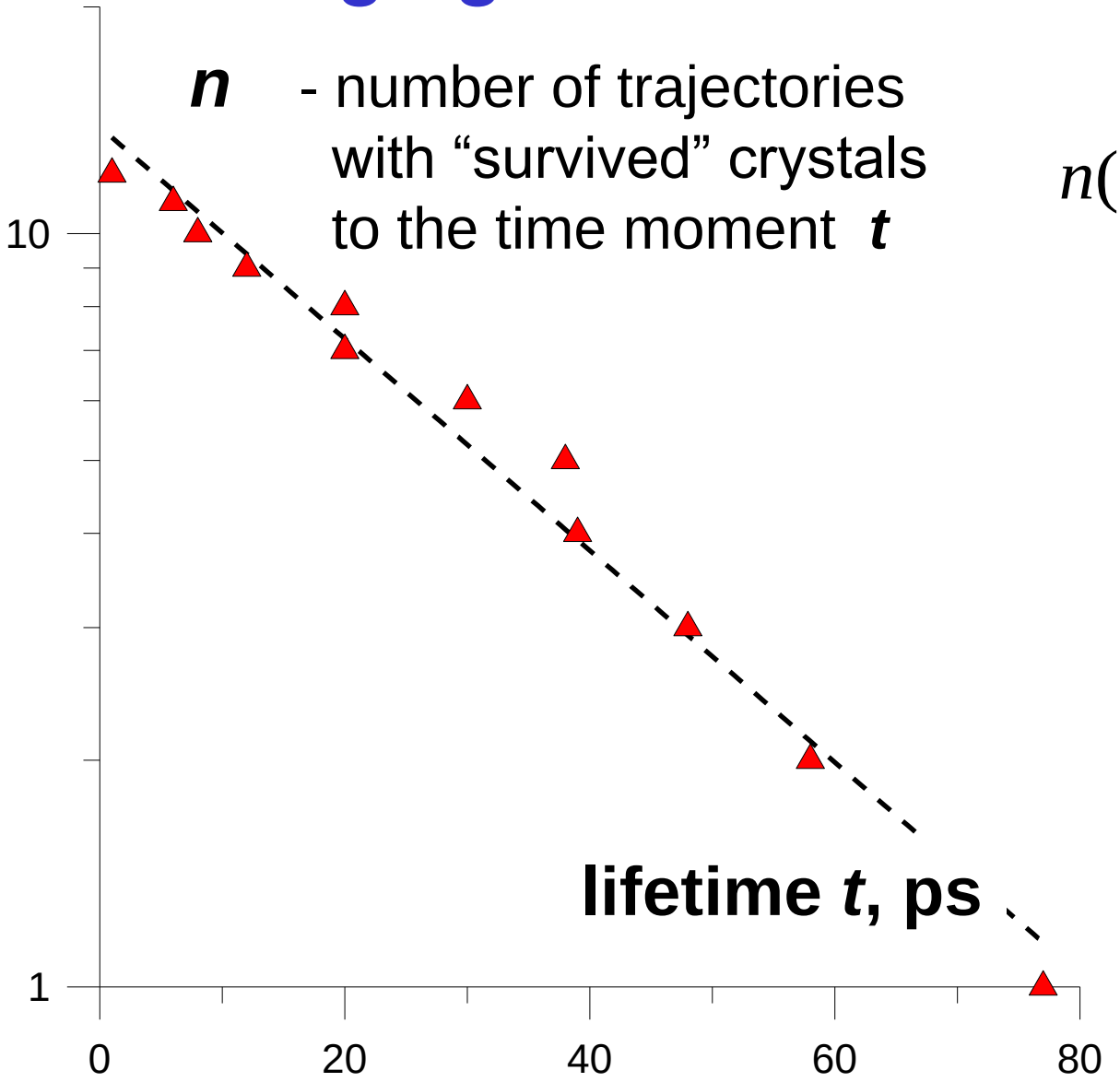




Calculation of nucleation rate: averaging over ensemble of MD runs

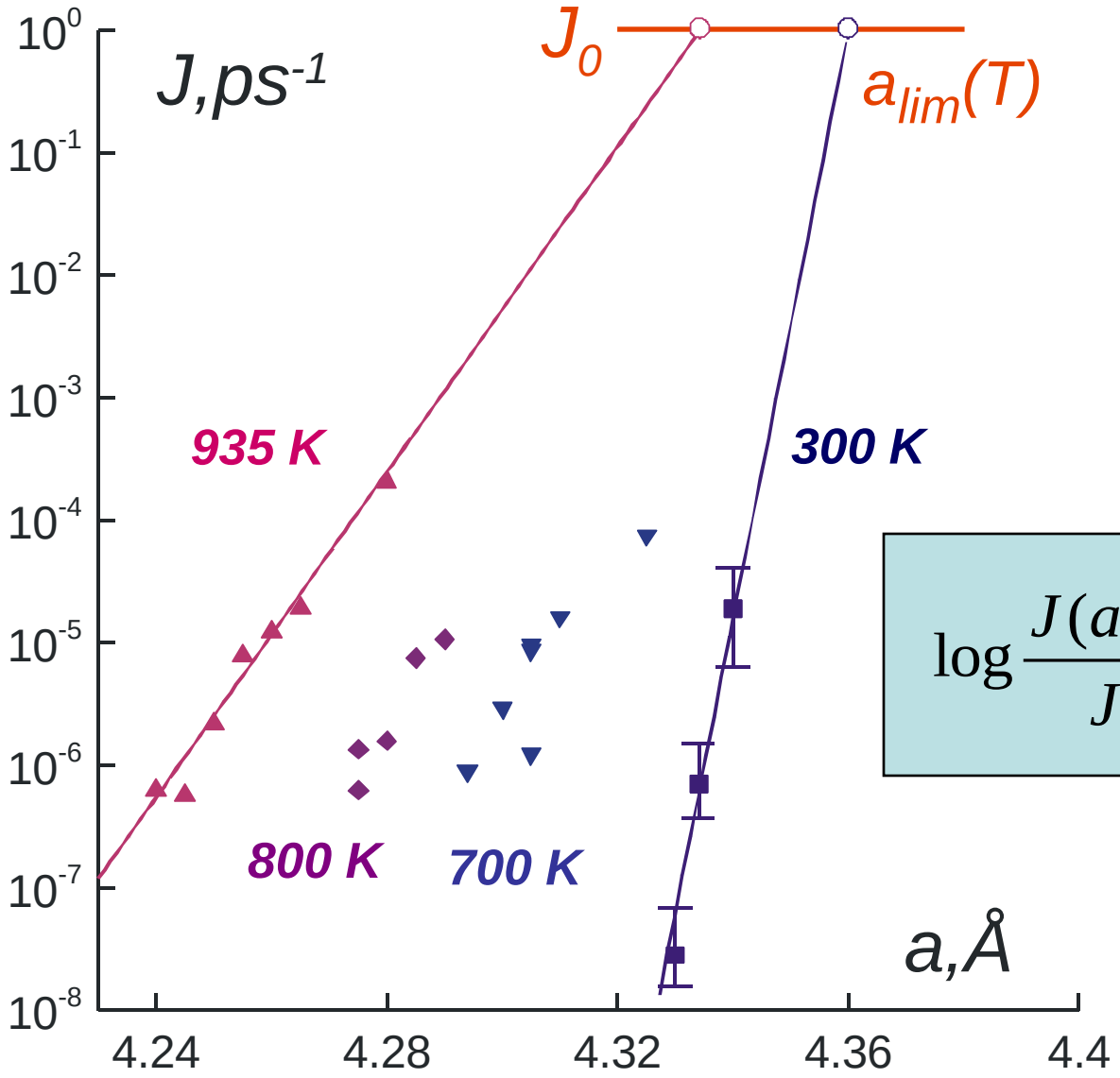
n - number of trajectories with “survived” crystals to the time moment ***t***

$$n(t) = n_0 \exp\left(-\frac{t}{\tau}\right)$$



$$J = \frac{1}{\langle \tau \rangle N}$$

Nucleation rate – lattice constant (J-a) dependence



$$\log \frac{J(a,T)}{J_o} = -A[a_{\lim}(T) - a]$$

Void nucleation rate

$$\log \frac{J(a,T)}{J_o} = -A[a_{\lim}(T) - a]$$

$$\dot{n}(a,T) = J(a,T)V_0$$

$$\boxed{\dot{n} = \dot{n}_0 \exp\left[-A(a_{\lim} - a)\right]}$$

NAG (Nucleation and Growth) Model
(Barbee T.W., Seaman J.L., Crewdson R.J. // Materials, 1972)

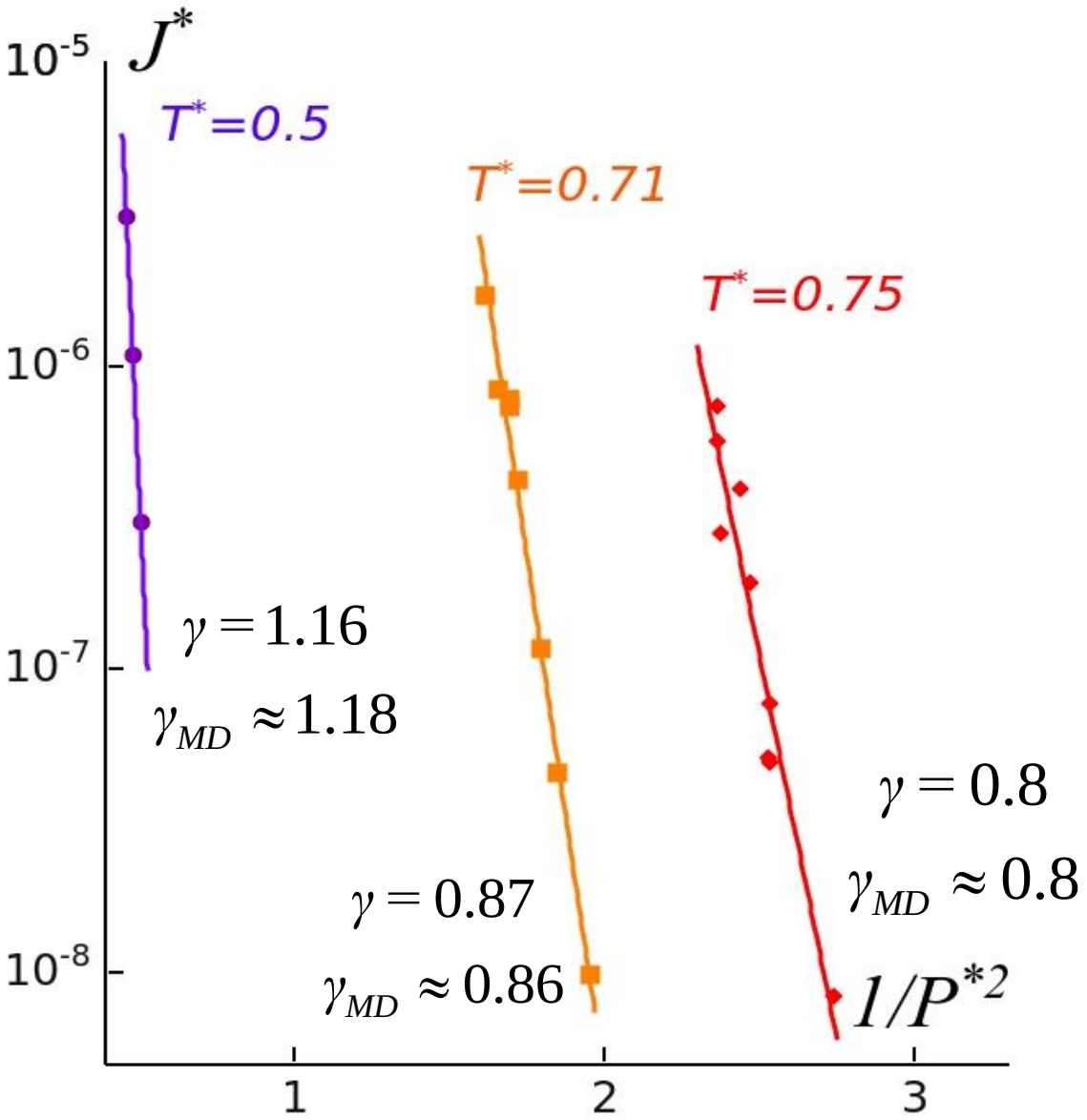
$$\dot{n}(\sigma) = \dot{n}_0 \exp\left(\frac{\sigma - \sigma_{n0}}{\sigma_1}\right)$$

threshold stress for nucleation

stress sensitivity

Nucleation rate: simple liquid

Dependence of void nucleation rate on pressure and temperature



$$J = \frac{1}{\langle t \rangle V}$$

$$J = J_0 \exp\left(-\frac{W}{k_B T}\right)$$

$$W = \frac{16\pi\gamma^3}{3\left(P - P'\right)^2}$$

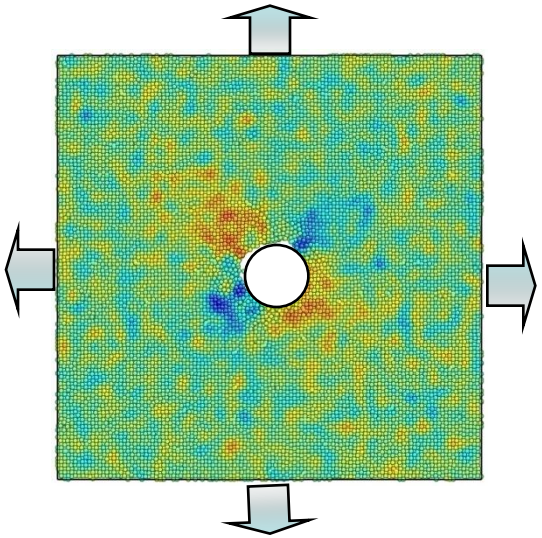
T = const:

$$\ln J = A - \frac{B}{P^2}$$

Void growth:
mechanisms of growth in crystals

Void growth mechanisms:

- **Migration of vacancies**



- **Elastic compression of media**

$$\sigma_r = p\left(1 - \frac{r_0^3}{r^3}\right) \qquad \sigma_\theta = p\left(1 + \frac{1}{2}\frac{r_0^3}{r^3}\right)$$

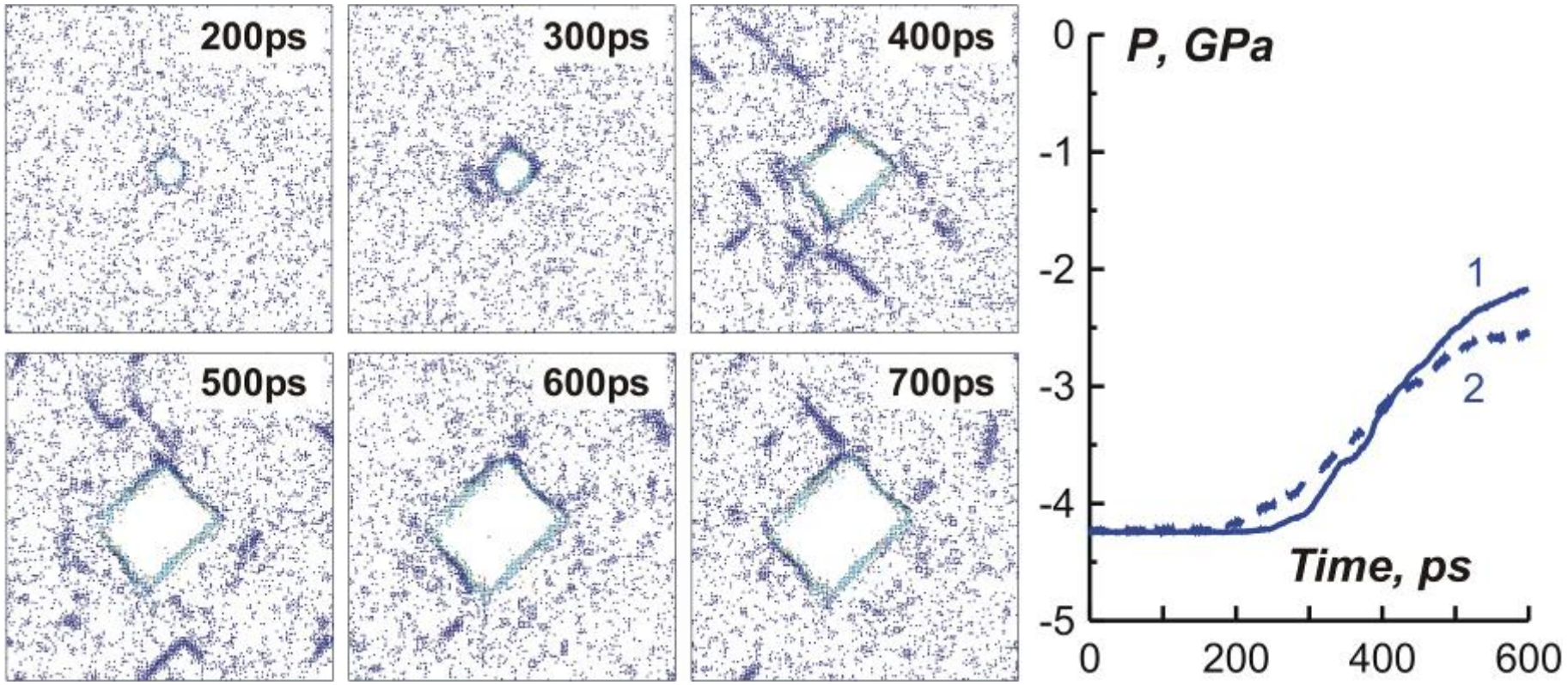
- **Plastic compression**

$$\frac{2}{3}\left(\sigma_r - \sigma_\theta\right) > Y$$

- **Melting + viscous growth**

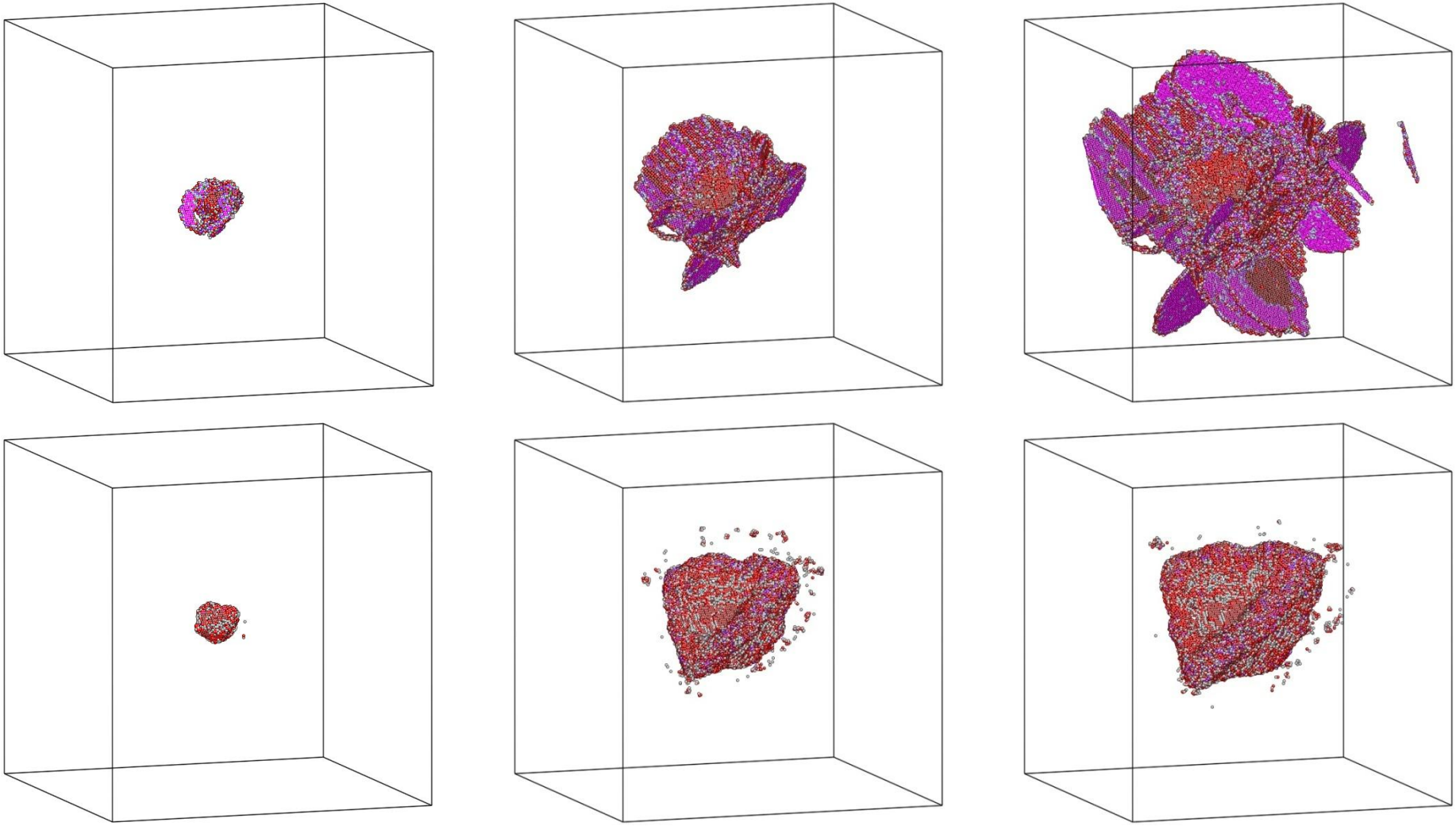
Spontaneous growth of void: emission of dislocation loops

700 K, 60x60x60, r_v=10Å, 700ps **Al***[Foiles]* *Relaxation*



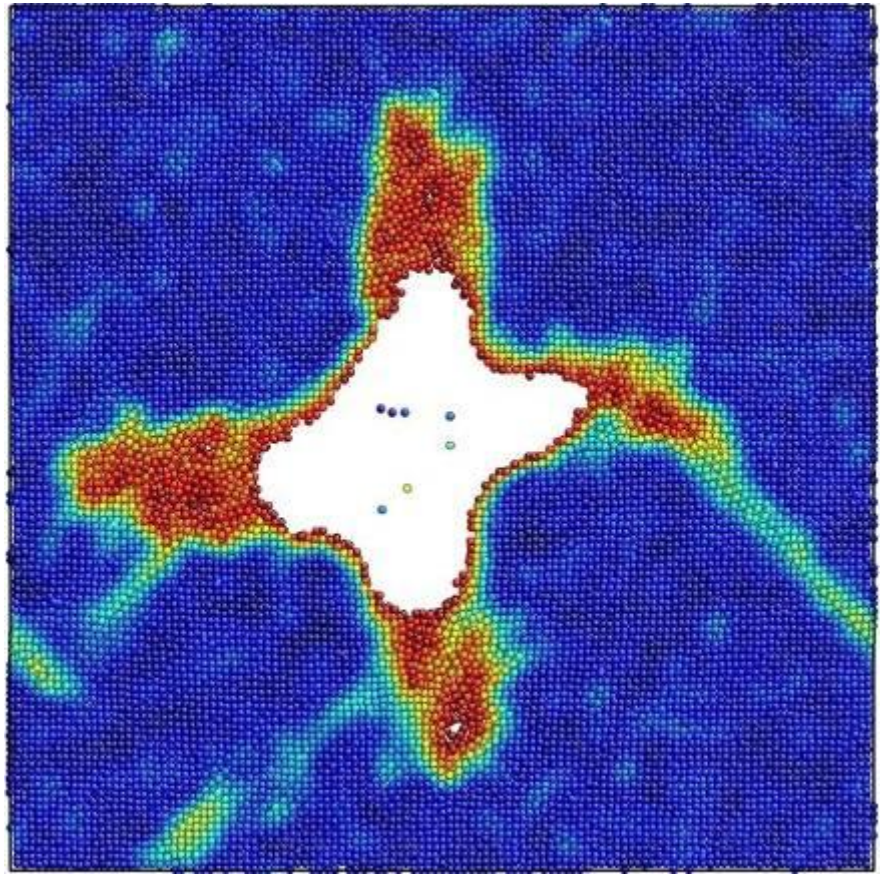
Spontaneous growth of void: shear loops

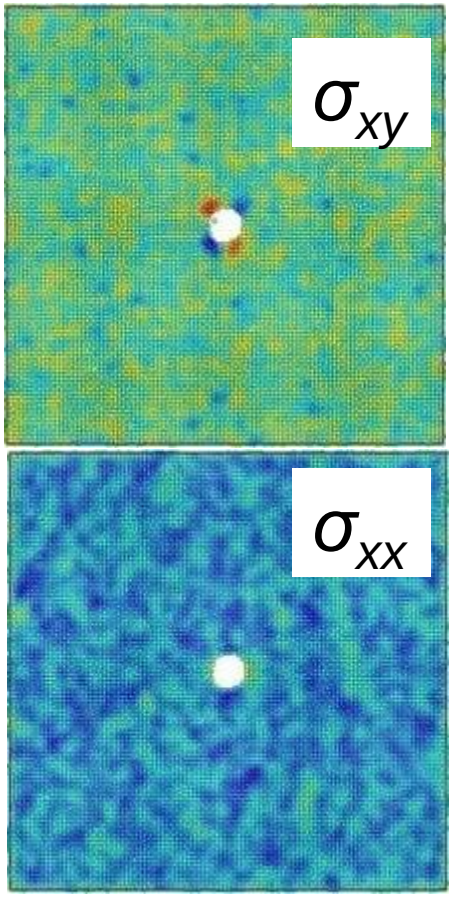
300 K, 100x100x100, r_v=10Å **Al***[Foiles]* *Relaxation*



Void growth: dislocations and amorpisation

- anisotropic distribution of local shear stresses
- void growth via emission of dislocation loops
- amorphisation of dislocation loops and their junctions

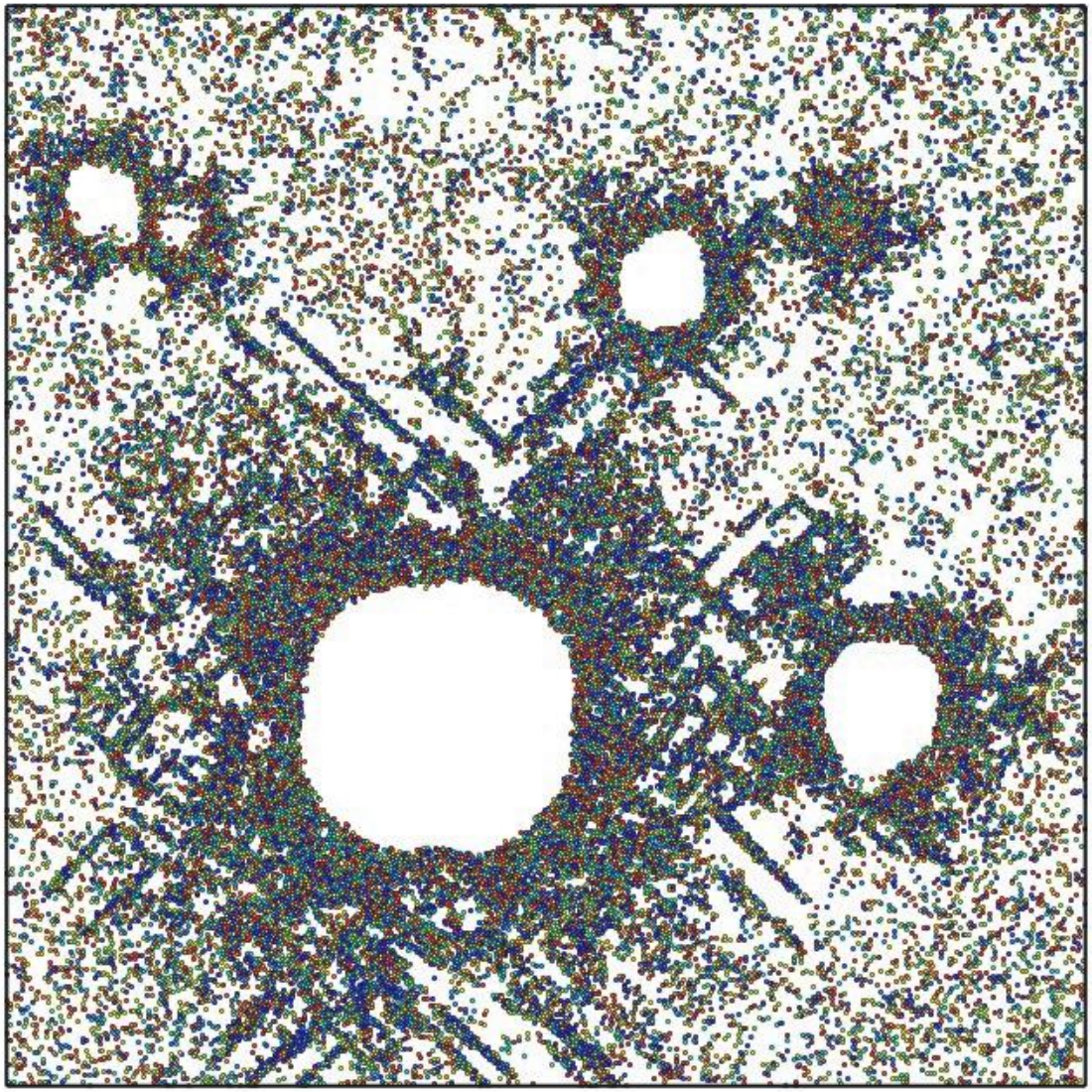




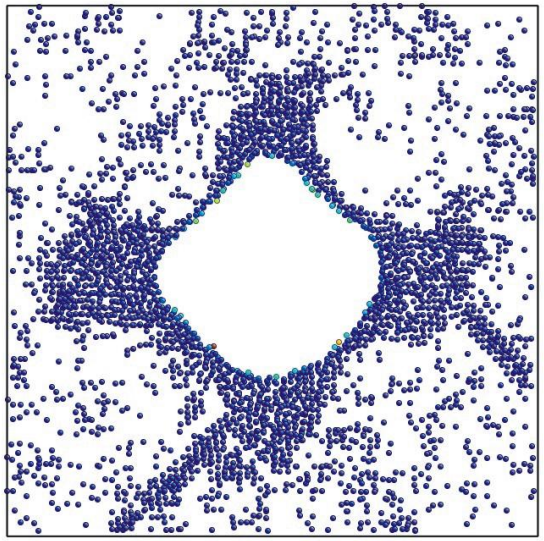
Al T_0=700K 250x250x250 A r_p=10 A $\dot{V}/V_0 = 10^8\ s^{-1}$

Influence of T and growth rate on amorphisation

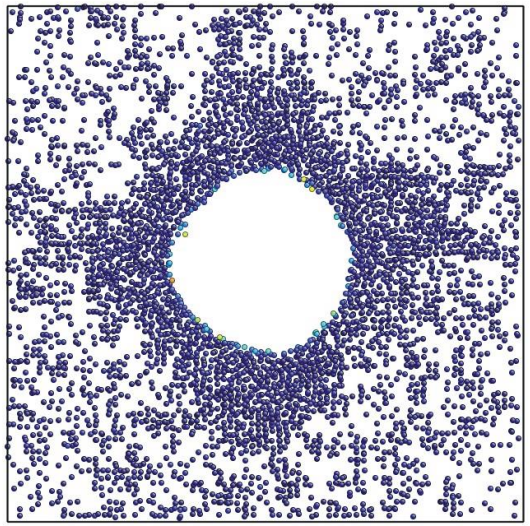
300 K, 200x200x20



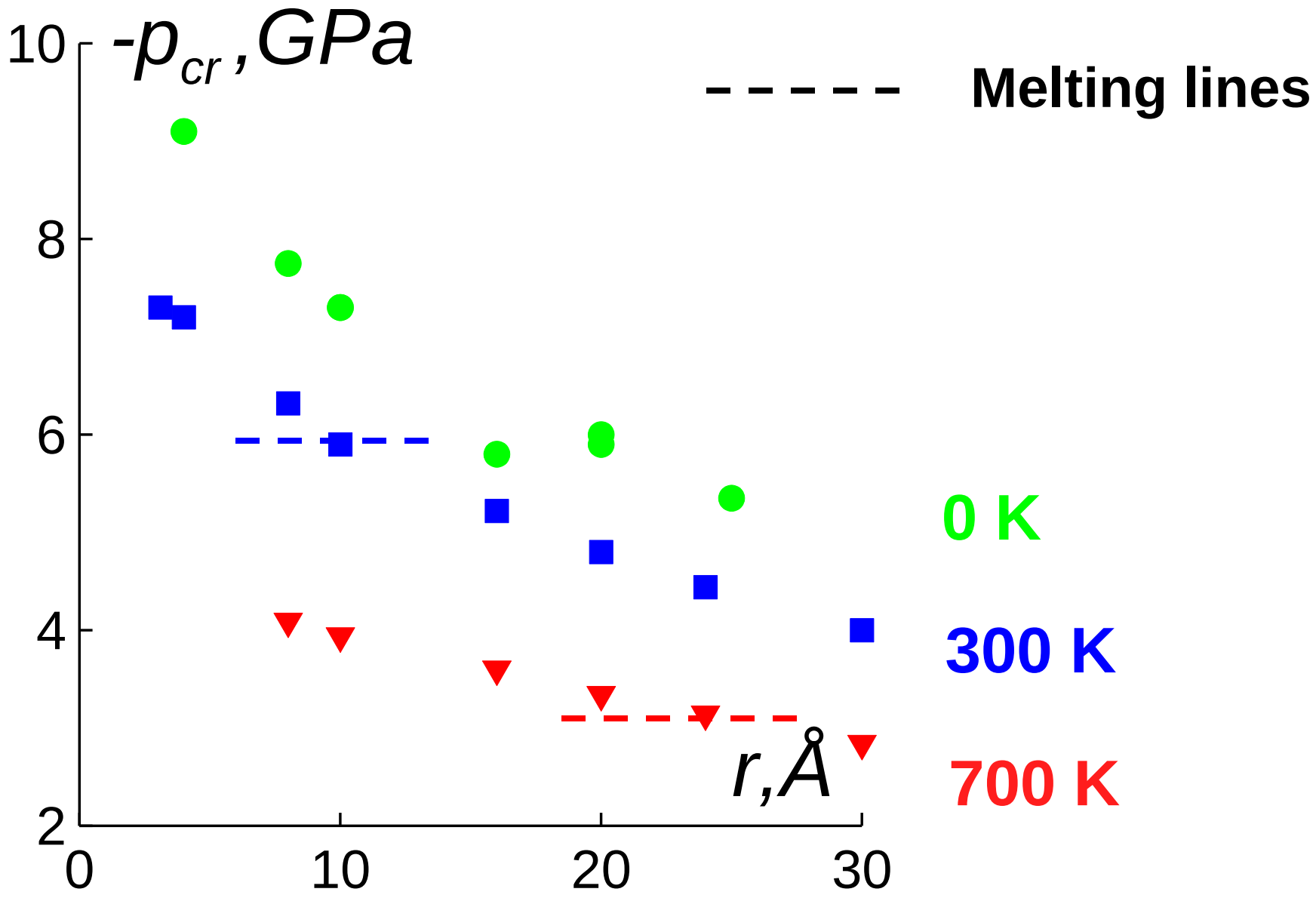
700 K, 40x40x40



900 K, 40x40x40



Crytical stress for void growth in Al



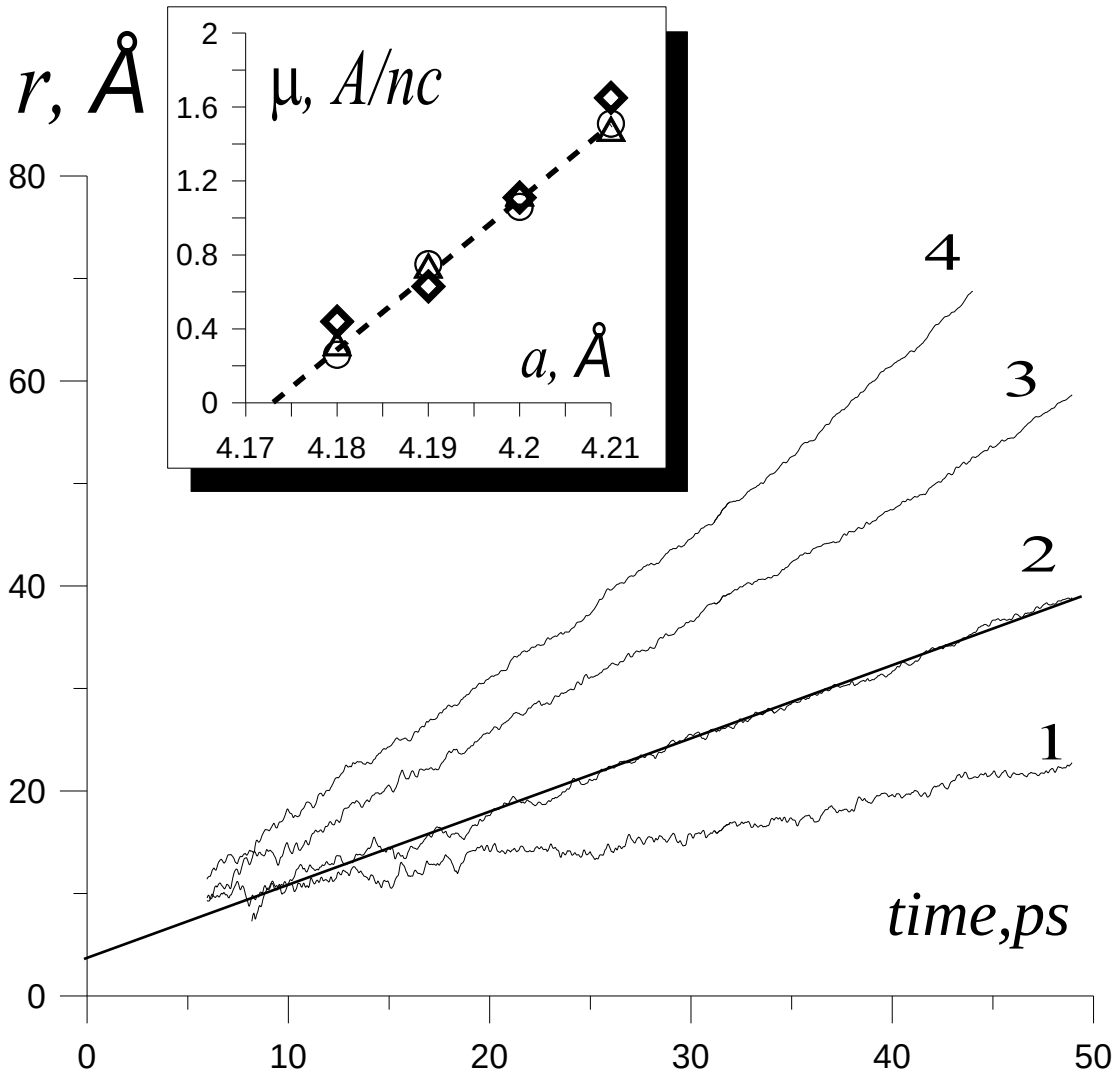
Void growth:
kinetics of growth in crystals

Void growth rate: calculation method

- System equilibration
- Spherical void cut out
- Evolution of void in the box with: constant volume or stress

$$r_{void}(t) \longrightarrow \mu = \dot{r}_{void}(t)$$

Dependence of growth rate on tensile stress and temperature



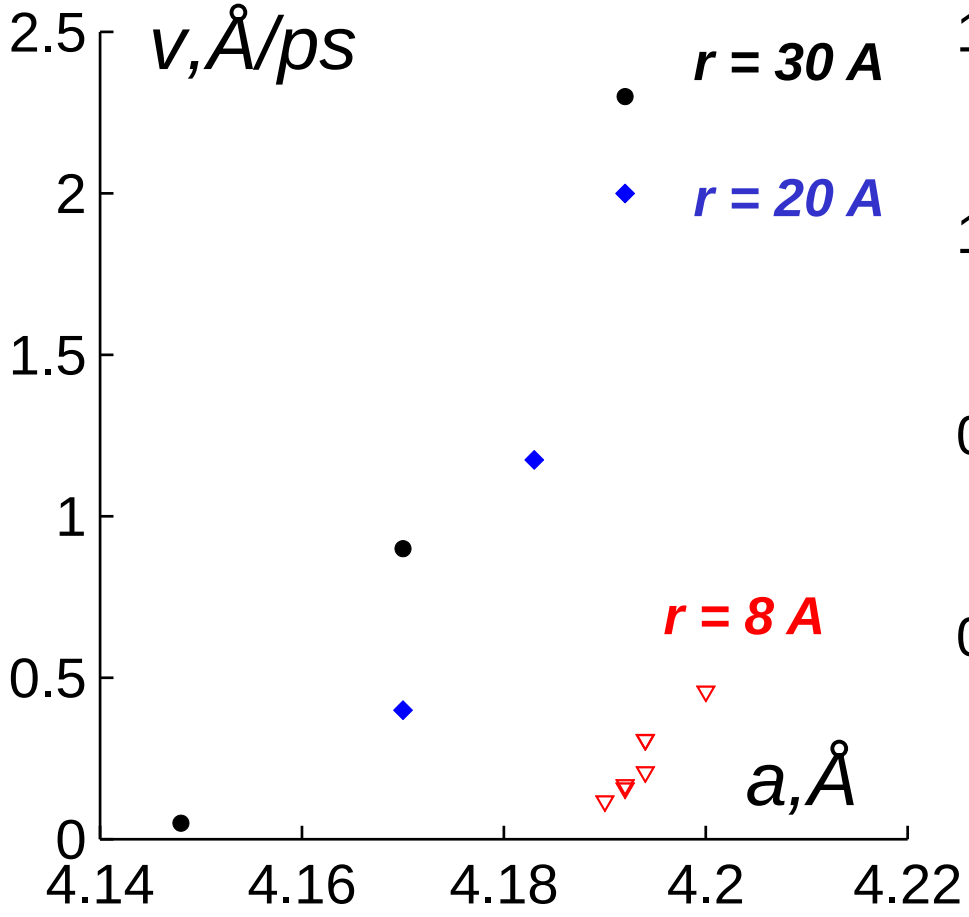
Lattice constant a:

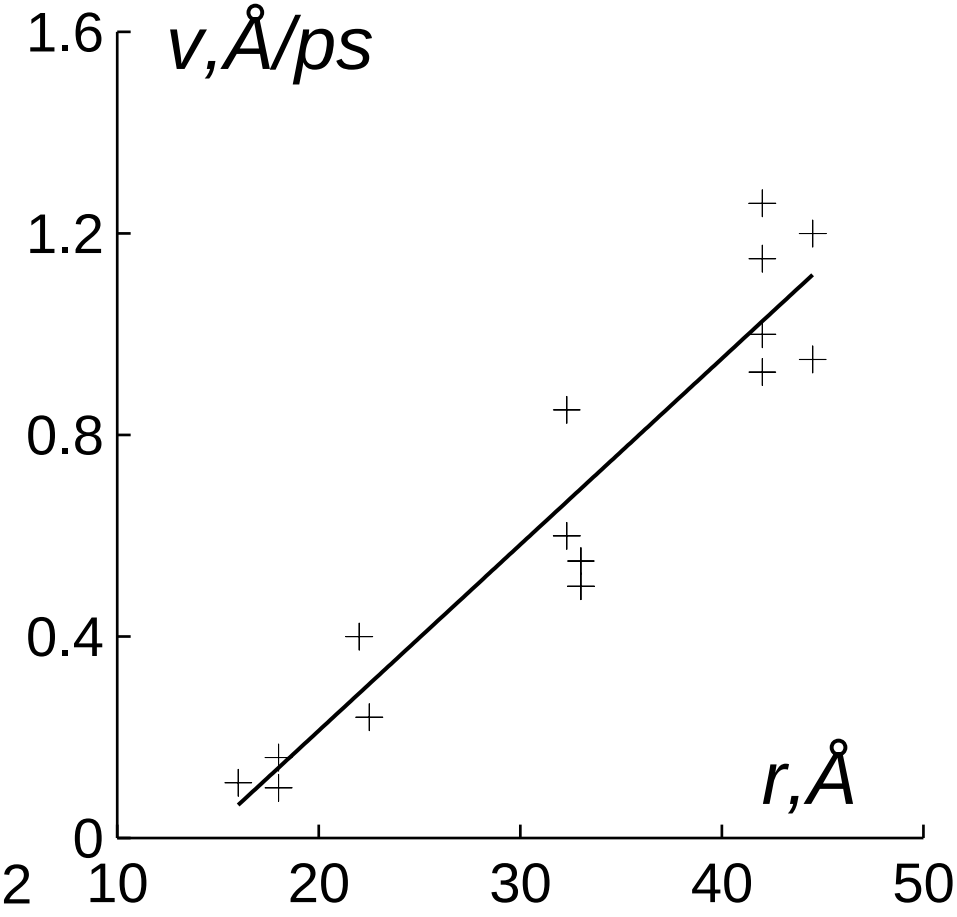
1 – 4.18 A
2 – 4.19 A
3 – 4.20 A
4 – 4.21 A

$$r(t) = r_0 + \mu t$$

$$r(t) = \int_0^t \mu\left[a(\tau)\right] d\tau$$

Dependence of growth rate on tensile stress and void radius





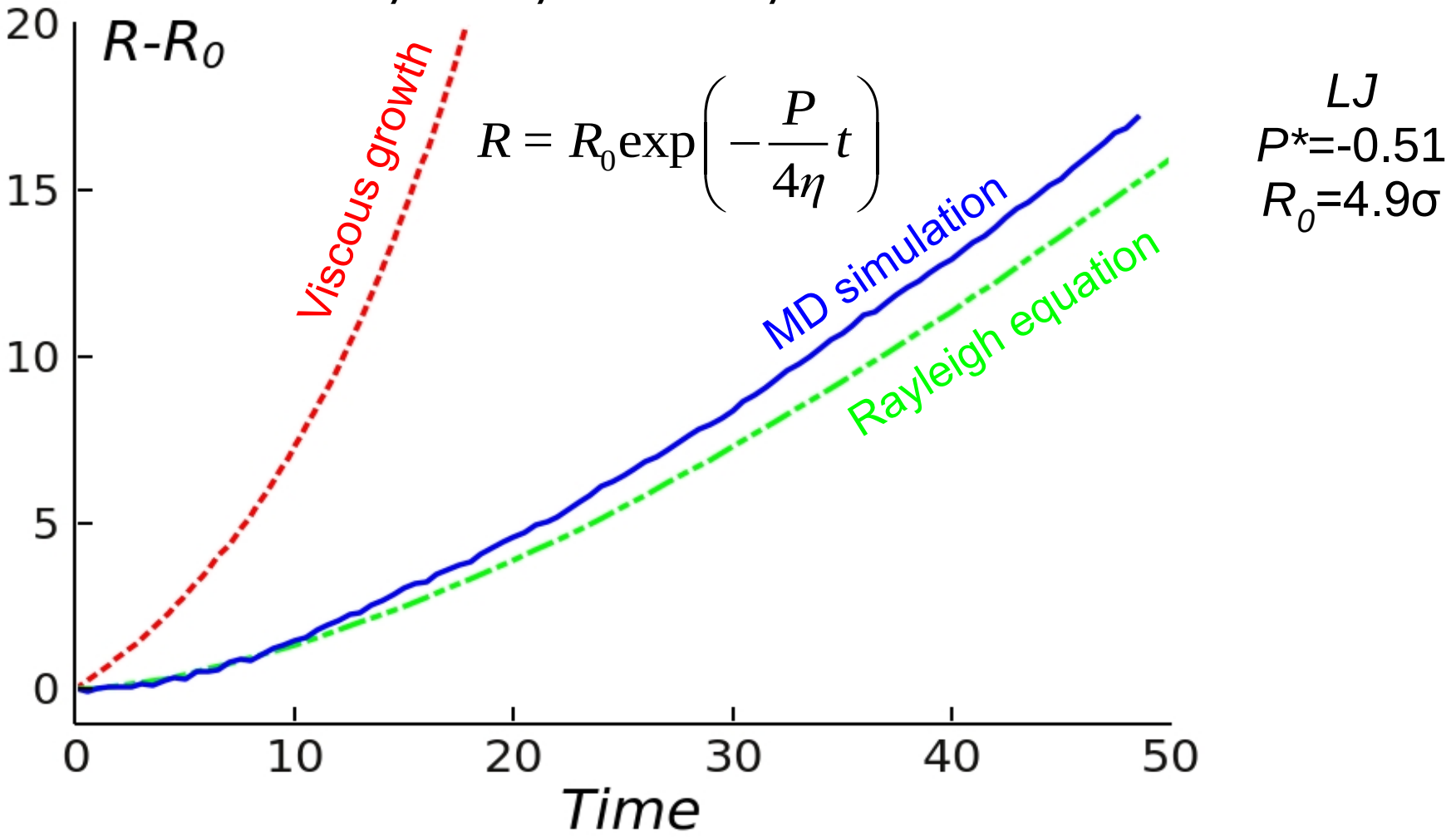
Al T = 700K 120x120x120 r_v = 8…40 A

Void growth:
kinetics of growth in liquids

Comparison of MD and hydrodynamics of incompressible liquid

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 + \frac{4\eta\dot{R}}{\rho R} + \frac{2\gamma}{\rho R} = -\frac{P_\infty(t)}{\rho}$$

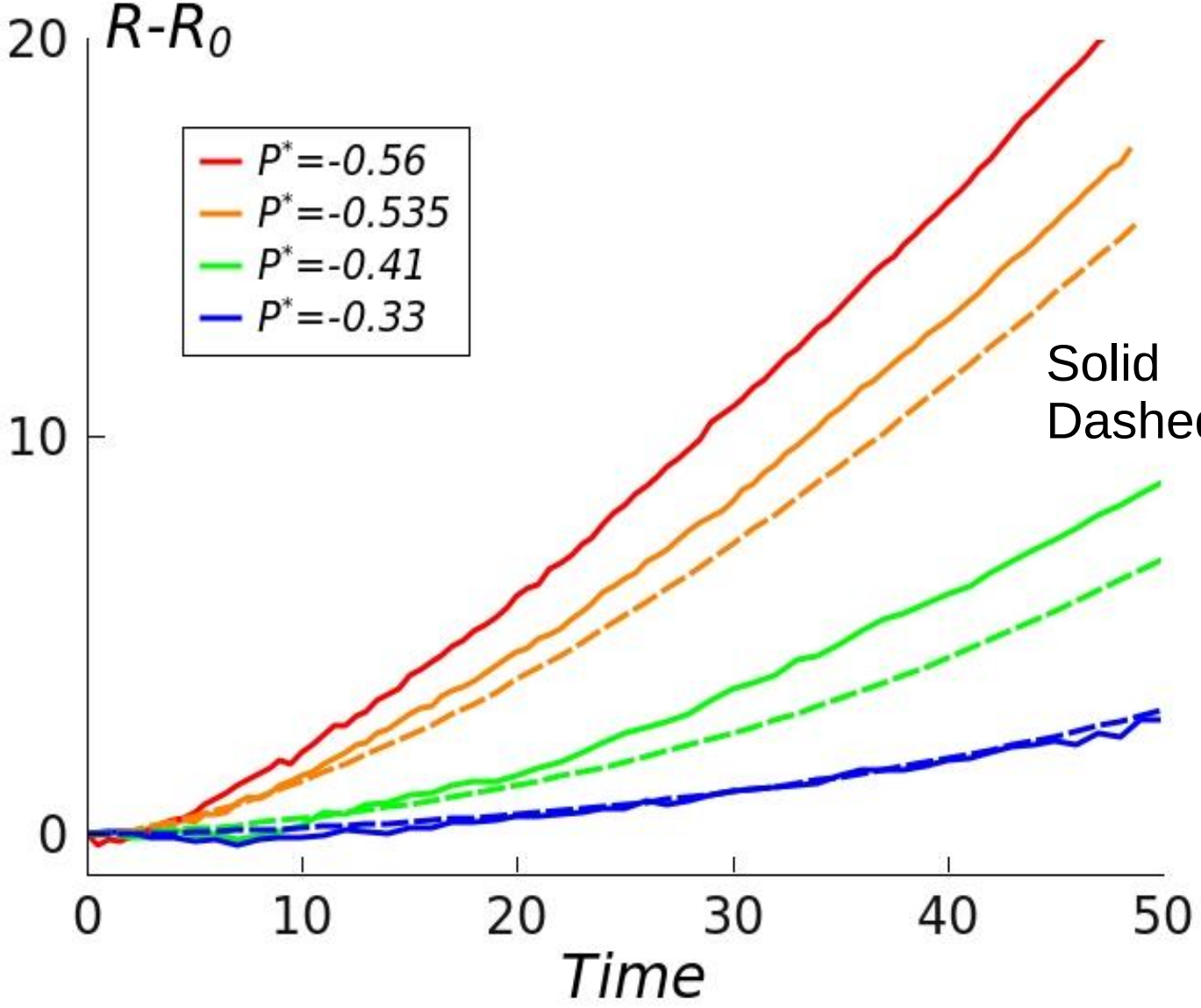
Rayleigh equation



$$R = R_0 \exp\left(-\frac{P}{4\eta}t\right)$$

LJ
*P**=-0.51
R_0=4.9σ

Comparison of MD and hydrodynamics of incompressible liquid



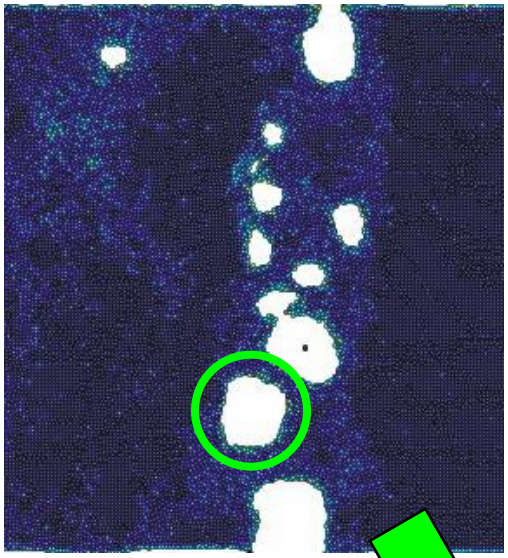
LJ
T^*=0.75

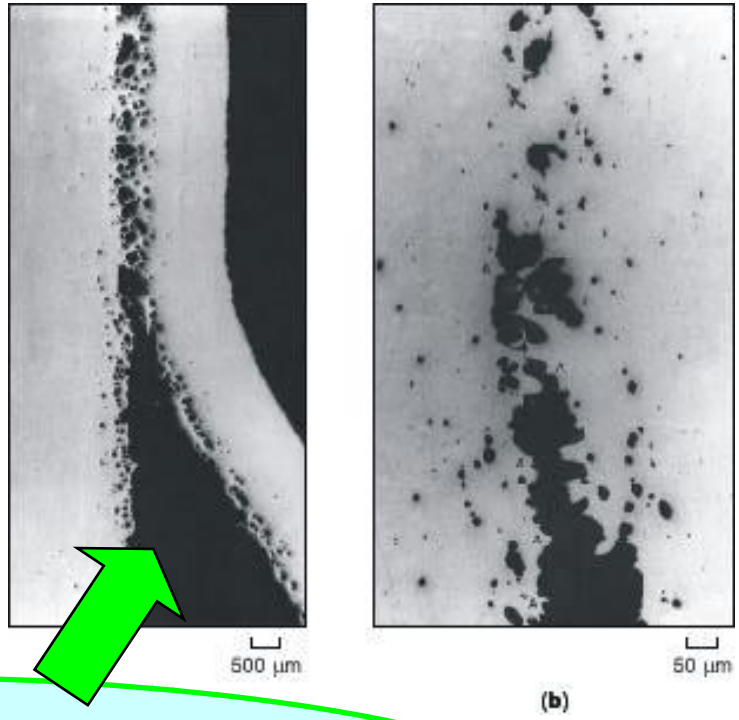
Lines:
Solid – MD simulation
Dashed – hydrodynamics

Kinetic Model of Fracture

Direct MD

Kinetic model





- Nucleation rate of voids J(a,T)
- Void growth rate μ(a,T)

- Straining history a(t), T(t)

Basic relations

Void's nucleation rate

$$\dot{n}(t) = J\left[a(t)\right]V_0$$

Volume of a void

$$v_{\mathrm{v}}(t) = \frac{4\pi}{3}\left(\int_0^t \mu\left[a(\tau)\right]d\tau\right)^3$$

Total volume of voids

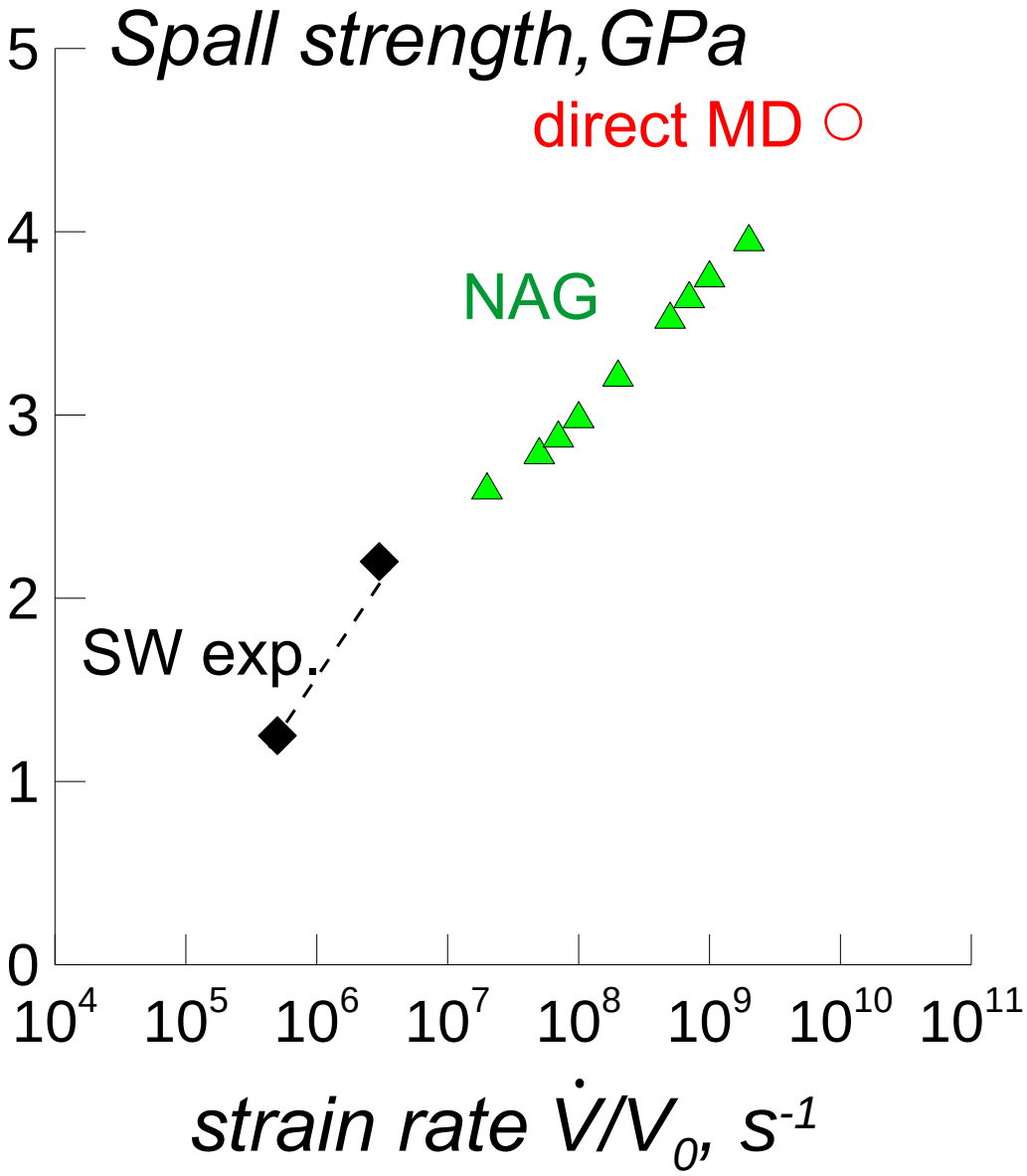
$$V_{\mathrm{v}} = \int_0^t v_{\mathrm{v}}(t-\tau)\dot{n}(\tau)d\tau$$

$$\frac{V_{\mathrm{v}}}{V_0} = \int_0^t \frac{4\pi}{3}\left(\int_\tau^t \mu\left[a(\xi)\right]d\xi\right)^3 J\left[a(\tau)\right]d\tau$$

Spallation criteria

$$V_{\mathrm{v}} = V_0 \longrightarrow t_{spall}$$

Estimation of the spall strength: *Al, T ≈ 900 K*

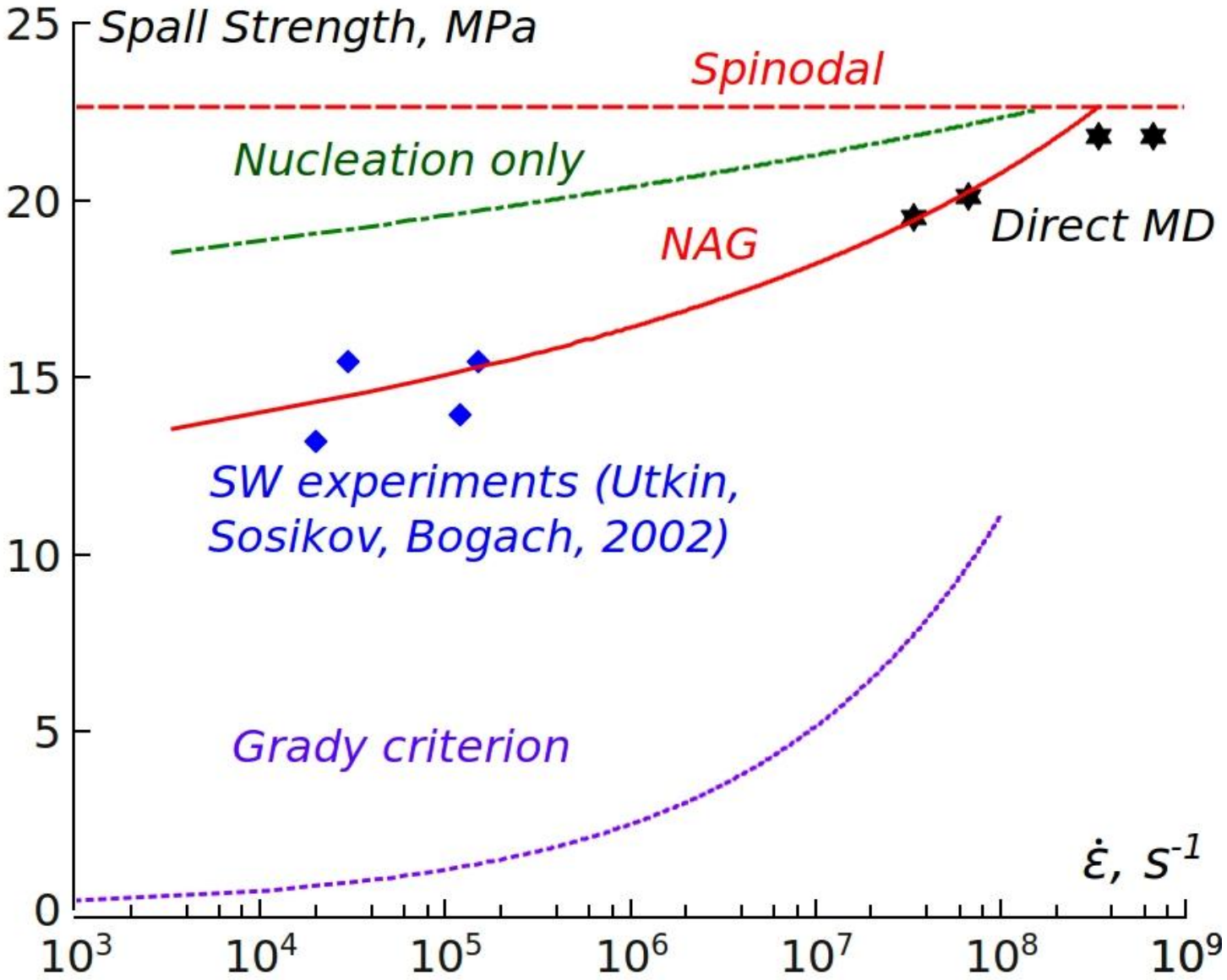


SW experiment:
Kanel, Razorenov, Baumung, Bluhm, 2001

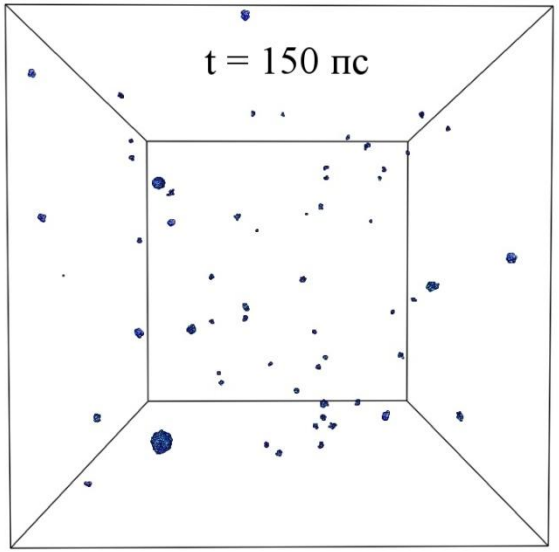
Al, T=900K

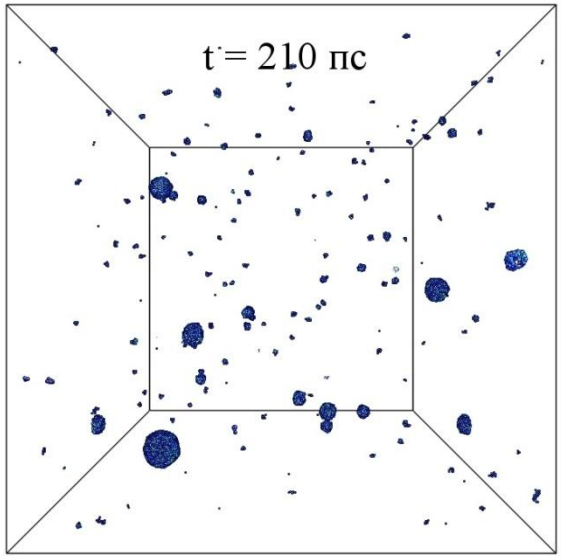
N ~ 10^6
N ~ 10^5

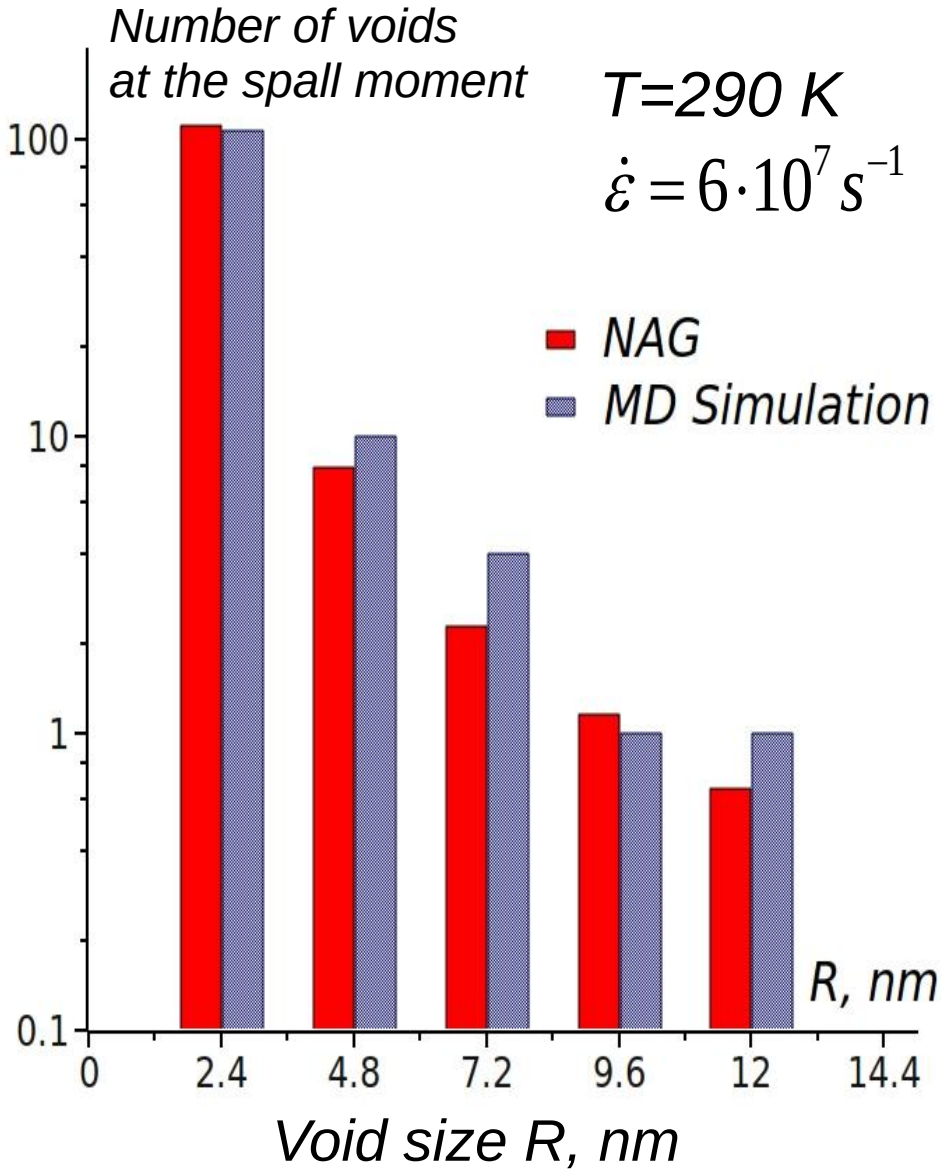
Estimation of the spall strength: hexane, $T \approx 300$ K



Fracture kinetics: Comparison of kinetic model with direct MD







Conclusions

- Kinetic model of fracture
  - ‘nucleation and growth’ approach
  - based on the results of MD simulations
  - estimations of spall strength
  - comparison with direct MD and experiments

- Single crystal - Al
  - void nucleation and growth rates from MD
  - void growth mechanism depends on T and strain rate
  - heterogeneous nucleation should be taken into account at low $T < 0.7\ T_m$

- Liquid - Hexane
  - nucleation rate can be fitted in the form of classic nucleation theory
  - Rayleigh equation is applicable for description of the growth kinetics of small voids