MULTISCALE INVESTIGATION OF DYNAMIC FRACTURE OF METALS AND METAL MELTS

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Copper plate after high-current electron irradiation

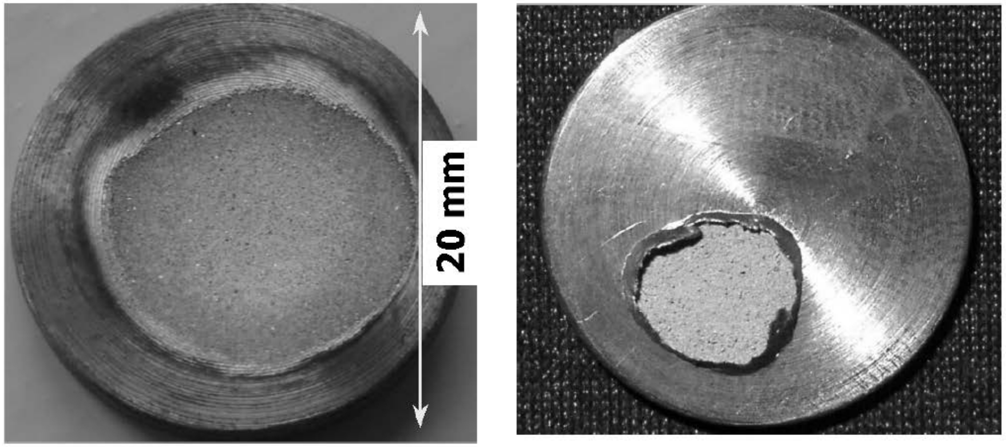


Fig. 3. Front (left) and rear (right) specimen surfaces upon a one-pass electron beam treatment

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)

Common framework

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

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

$\mathbf{w}$ plastic deformation tensor $\mathbf{S}$ tensor of stress deviators

Krasnikov V.V., Mayer A.E., Yalovets A.P. // Int. J. Plast. (2011)
Mayer A.E., Khishchenko K.V., Levashov P.R., Mayer P.N. // J. Appl. Phys. (2013)
Borodin E.N., Mayer A.E. // Int. J. Plast. (2015)

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

Fracture model

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

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

Model of fracture

Spherical pores

$$\mathbf{W} = \begin{pmatrix} W/3 & 0 & 0 \\ 0 & W/3 & 0 \\ 0 & 0 & W/3 \end{pmatrix}$$

$$W = \ln(1-\alpha)$$

$$\alpha = \sum_{m=1}^{M} \left(\frac{4\pi}{3} R_m^3 n_m \right)$$

suppose that all spherical voids have the same (mean) radius $\alpha = \frac{4\pi}{3} R^3 n$

equation for mean radius

$$\frac{dR}{dt} = \left(\dot{R}\right)_p - \left(R - R_c^3 / R^2\right)\dot{n}/n$$

$\left(\dot{R}\right)_p$ growth rate of particular void with mean radius R_c critical void radius

total concentration of voids

$$\frac{dn}{dt} = \left[(\dot{n})_1 + (\dot{n})_2\right](1-\alpha) - n(\nabla \cdot \mathbf{v})$$

$(\dot{n})_1$ nucleation of new voids $(\dot{n})_2$ activation of pre-existing pores

Metal melts

Molten metal: continuum model

$$\frac{d}{dt}\left(\dot{R}\right)_p = -\frac{3}{2}\frac{1}{R}\left(\left(\dot{R}\right)_p\right)^2 + \frac{1}{R\rho}\left[-P - \frac{2\sigma}{R}\right] - \frac{2}{3}\frac{\eta}{\rho}\frac{1}{R^2}\left(\dot{R}\right)_p$$

Rayleigh-Plesset equation

$$\left(\dot{n}\right)_1 = \frac{c}{a^4}\cdot\exp\left(-\frac{16\pi\gamma^3}{3kT\cdot P^2}\right)\cdot\left(1-\alpha\right)$$

rate of nucleation

$$\left(\dot{n}\right)_2 = 0$$

Surface tension

$$\gamma\left(R,T\right) = \gamma'\left(T\right)/\left[1+\delta\cdot a/R\right]$$

$$\gamma'\left(T\right) = \gamma_m - K_\sigma\cdot\left(T-T_m\right)$$

[H.M. Lu, Q. Jiang // J. Phys. Chem. B (2005)]

$$K_\sigma = \sigma_m/\left(T_K - T_m\right)$$

a mean interatomic distance

Viscosity

$$\eta = 0.1\,\mathrm{mPa\times s}$$

EOS

Cu, Al, Fe, Pb [S.N. Kolgatin, A.V. Khachatur'yants // Teplofiz. Vys. Temp (1982)]

Ni, Ti [V.E. Fortov, K.V. Khishchenko, P.R. Levashov, I.V. Lomonosov // Nucl. Instrum. Meth. A (1998)]

Molten metal: molecular dynamics

LAMMPS [S. Plimpton // J. Comp. Phys. (1995) http://lammps.sandia.gov]

periodic boundary conditions

system in thermostat at constant temperature $T = \text{const}$

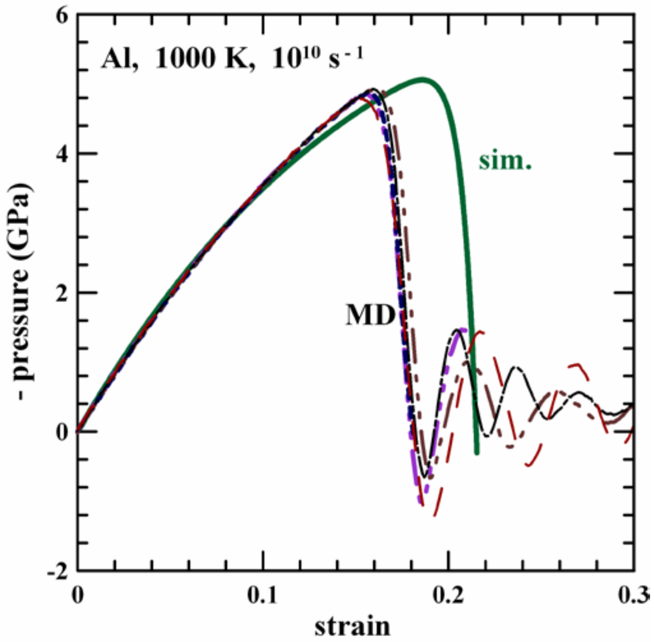
uniaxial tension with a constant rate of change of volume

$$\dot{V}(t) = \dot{\varepsilon} \cdot V_0$$

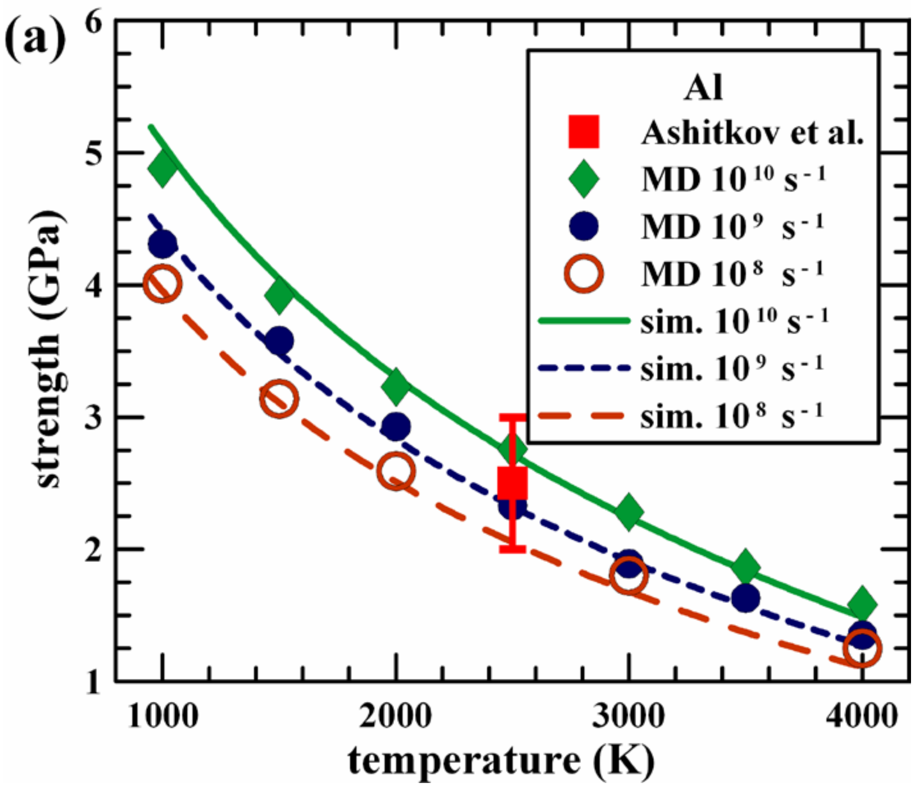
Interatomic potentials

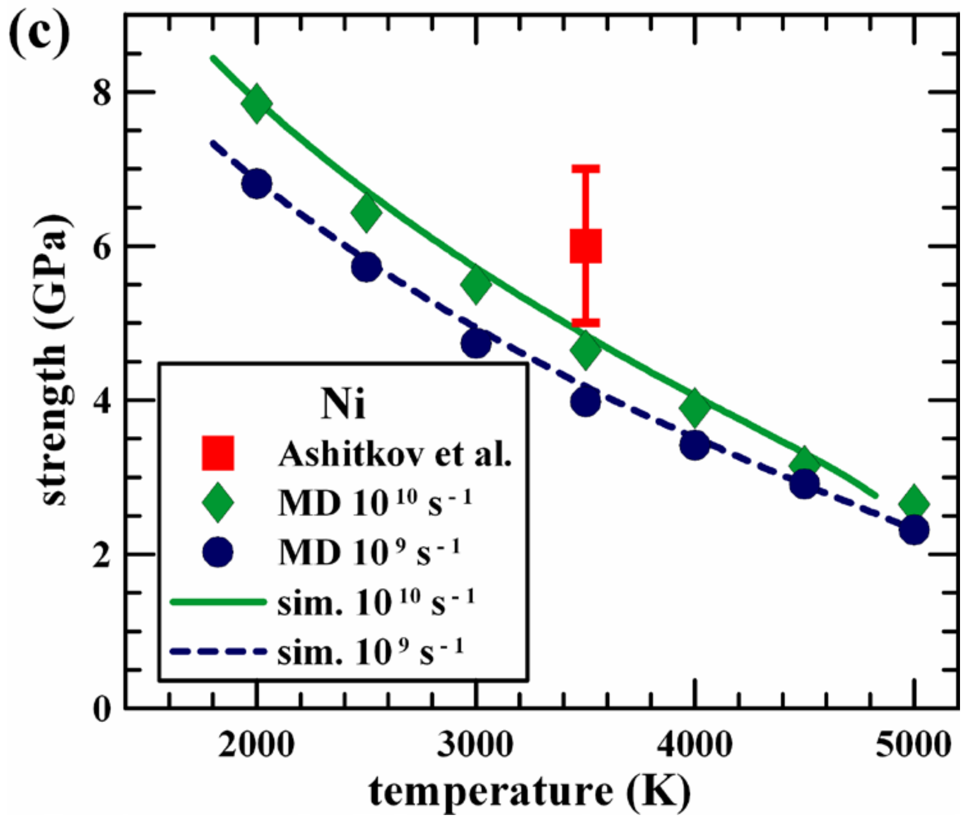
Al, Cu [X.W. Zhou, et al. // Acta mater. (2001)]

Fe, Pb, Ni, Ti [X.W. Zhou, R.A. Johnson, H.N.G. Wadley // Phys. Rev. B. (2004)]



Temperature dependence of tensile strength (metal melt)





Experimental data:
S.I. Ashitkov, P.S. Komarov, A.V. Ovchinnikov, E.V. Struleva, N.A. Inogamov, V.A. Khokhlov, V.V. Zhakhovsky, Yu.N. Emirov, I.I. Oleynik, M.B. Agranat (JIHT of RAS, Moscow, 2012).

Mayer A.E., Mayer P.N. // J. Appl. Phys. (2015) http://dx.doi.org/10.1063/1.4926861

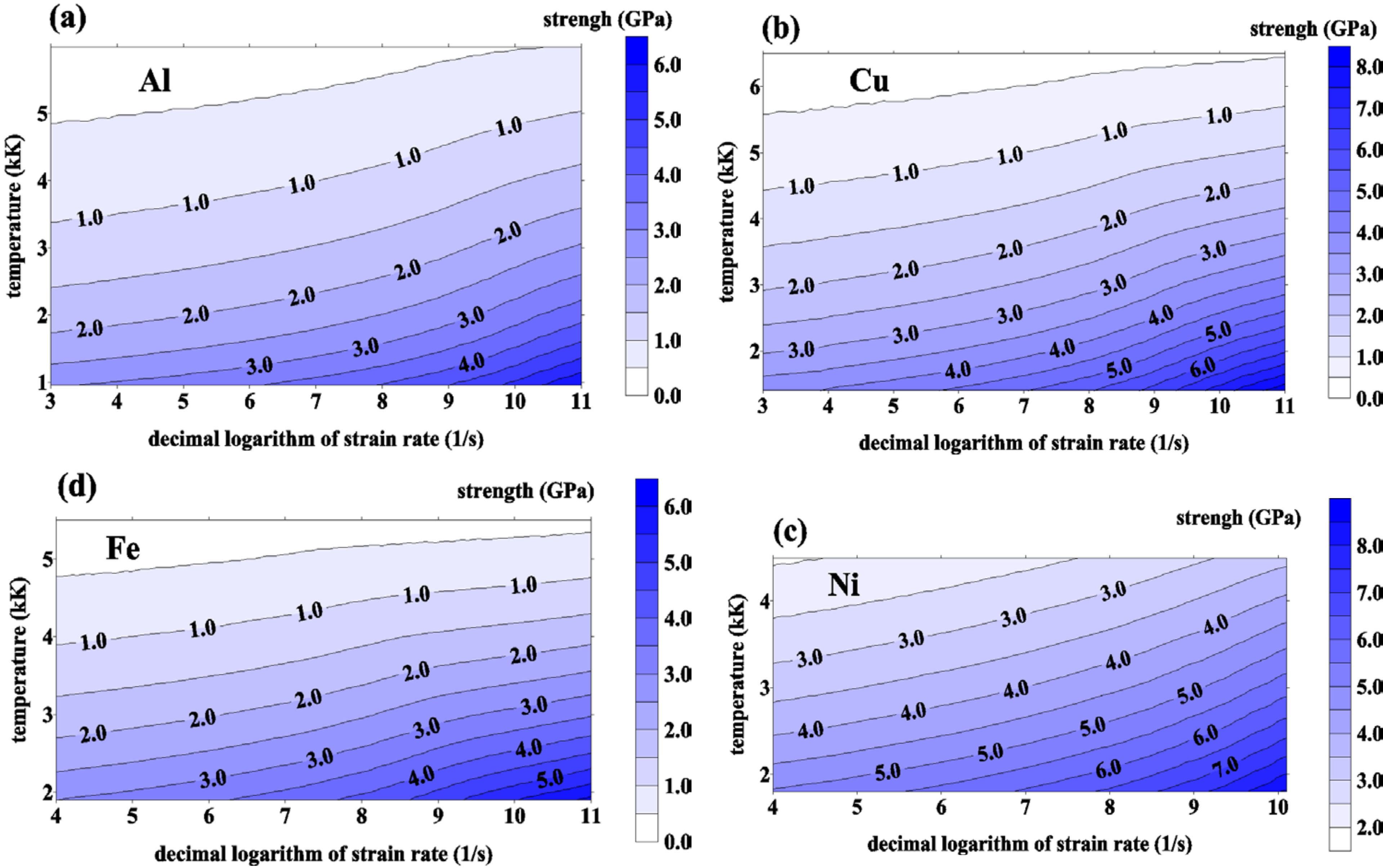
Parameters of the continuum model for metal melt

Parameter	Al	Cu	Ni	Fe	Ti	Pb
γ_m (J/m^2)	1.03	1.35	1.80	1.18	1.52	0.42
K (mJ/(m^{2}K))	0.15	0.21	0.23	0.26	0.20	0.12
δ	0.8	0.8	1.0	0.8	1.5	0.8
T_m (K)	933	1358	1728	1830	1940	601
η (mPa$\times$s)	0.1					

Surface tension coefficients from **[H.M. Lu, Q. Jiang // J. Phys. Chem. B (2005)]**

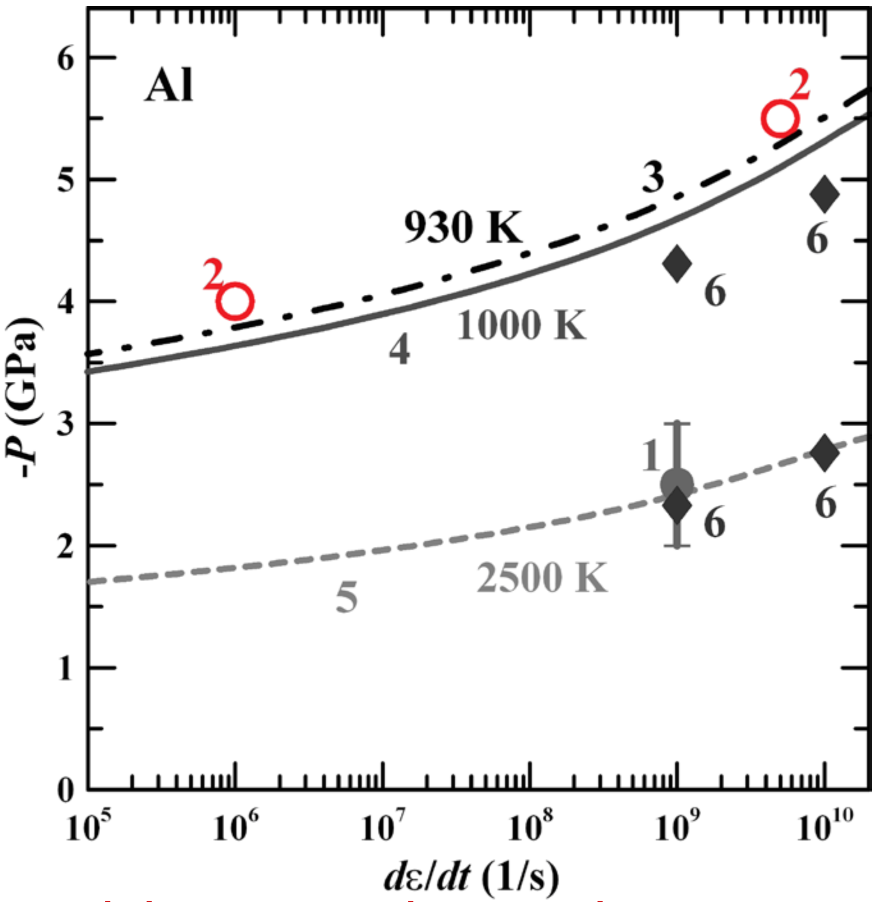
Mayer A.E., Mayer P.N. // J. Appl. Phys. (2015) http://dx.doi.org/10.1063/1.4926861

Maps of tensile strength

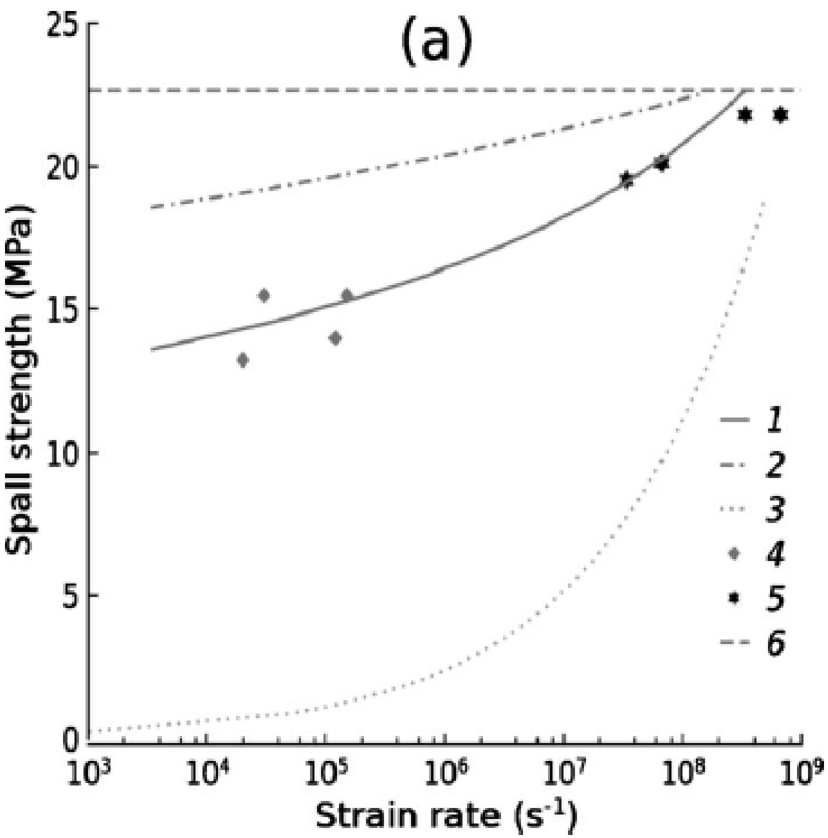


Mayer A.E., Mayer P.N. // J. Appl. Phys. (2015) http://dx.doi.org/10.1063/1.4926861

Strain rate dependences given by other models



Hexan (as a Lennard-Jones liquid)



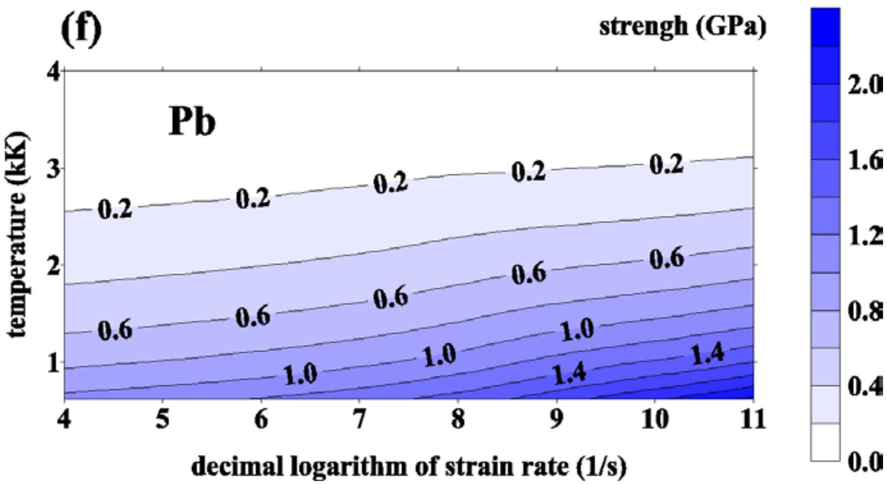
Kuksin A.Yu., Levashov P.R., Pisarev V.V., Povarnitsyn M.E., Yanilkin A.V., Zakharenkov A.S., // Physics of Extreme States of Matter – 2011 , (2011) Fortov V.E., et al (Eds.), IPCP RAS, Chernogolovka

Kuksin A.Yu., Norman G.E., Pisarev V.V., Stegilov V.V., Yanilkin A.V. // Phys. Rev. B (2010)

Mayer P.N. , Mayer A.E. // J. Exp. Theor. Phys. (2015)
http://dx.doi.org/10.1134/S1063776115060096

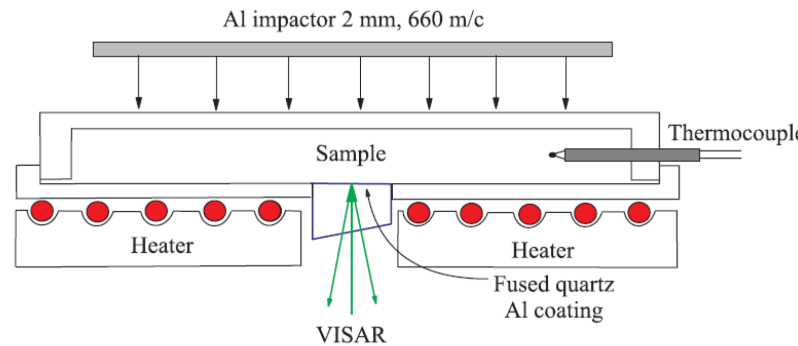
Strain rate dependences given by other models

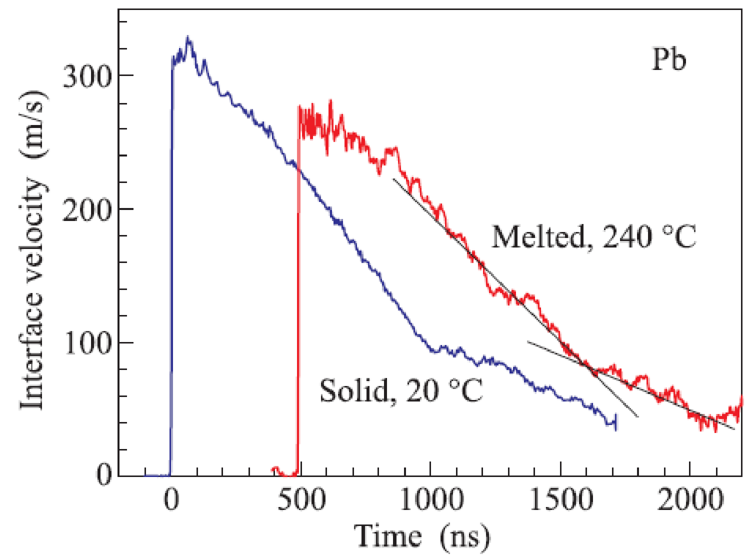
Continuum model based on
MD simulations



Mayer A.E., Mayer P.N. // J. Appl. Phys. (2015)
http://dx.doi.org/10.1063/1.4926861

High-velocity impact





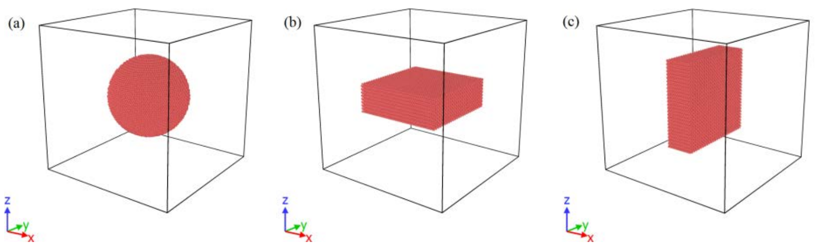
=> strength is less than 0.03 GPa

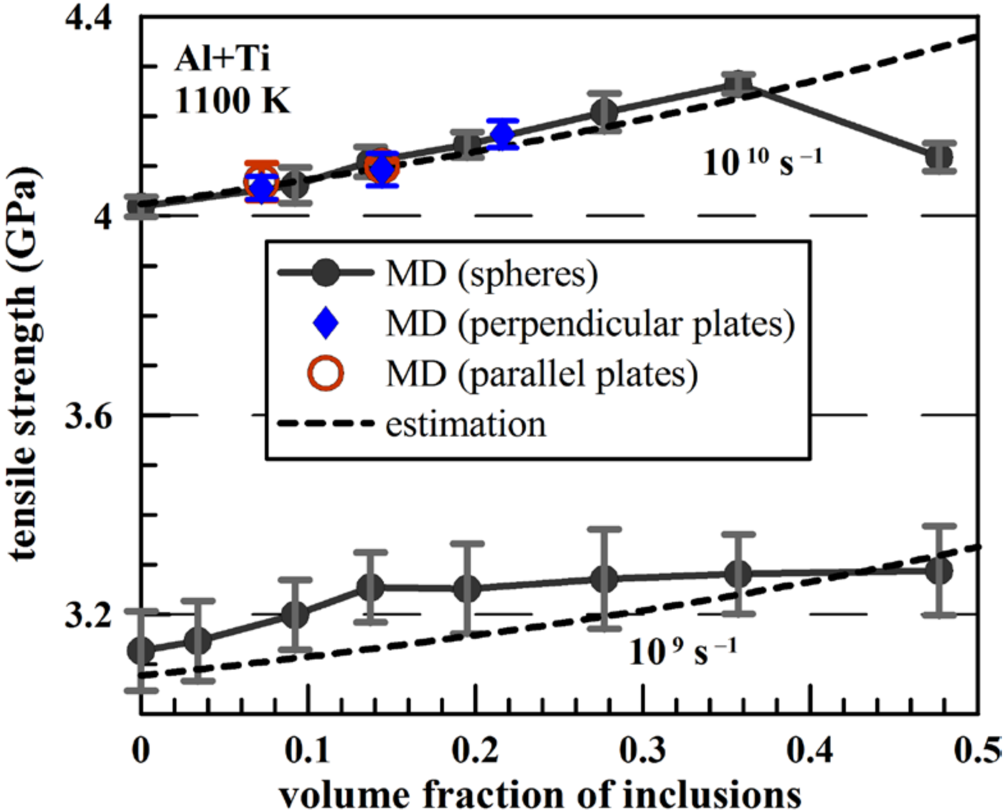
Kanel G.I. , Savinykh A.S., Garkushin G.V., Razorenov S.V. // JETP Lett. (2015).

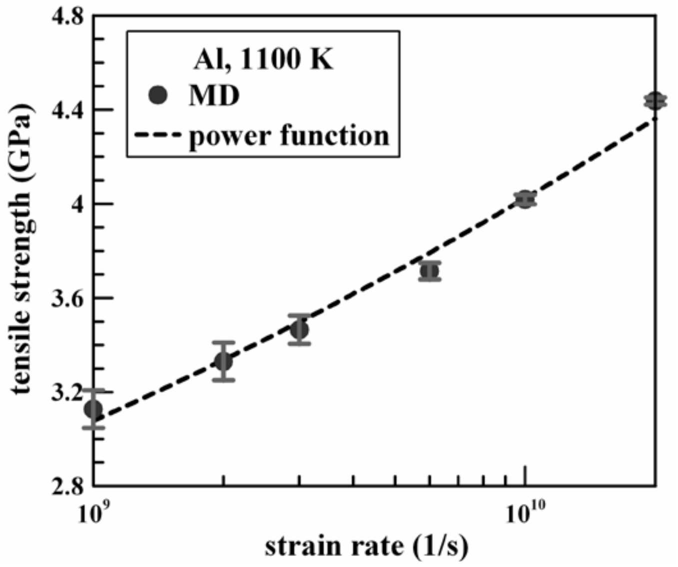
Refractory inclusions

Interatomic potential:
Al+Ti **[Zope R.R., Mishin Y. // Phys. Rev. B (2003)]**

Ti inclusions in Al melt







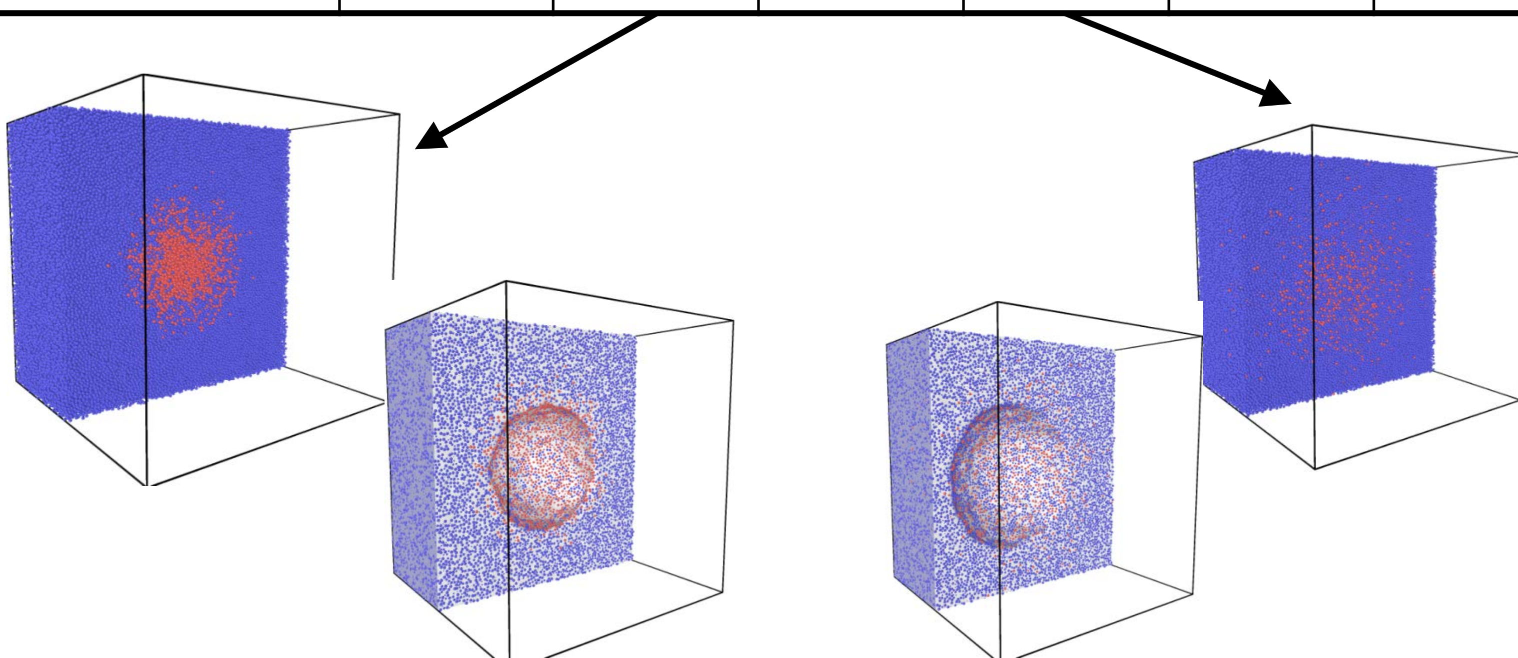
Hard refractory inclusions slightly increase the tensile strength !!!

Mayer A.E., Mayer P.N. // Comp. Mat. Sci. (2016)
http://dx.doi.org/10.1016/j.commatsci.2015.12.040

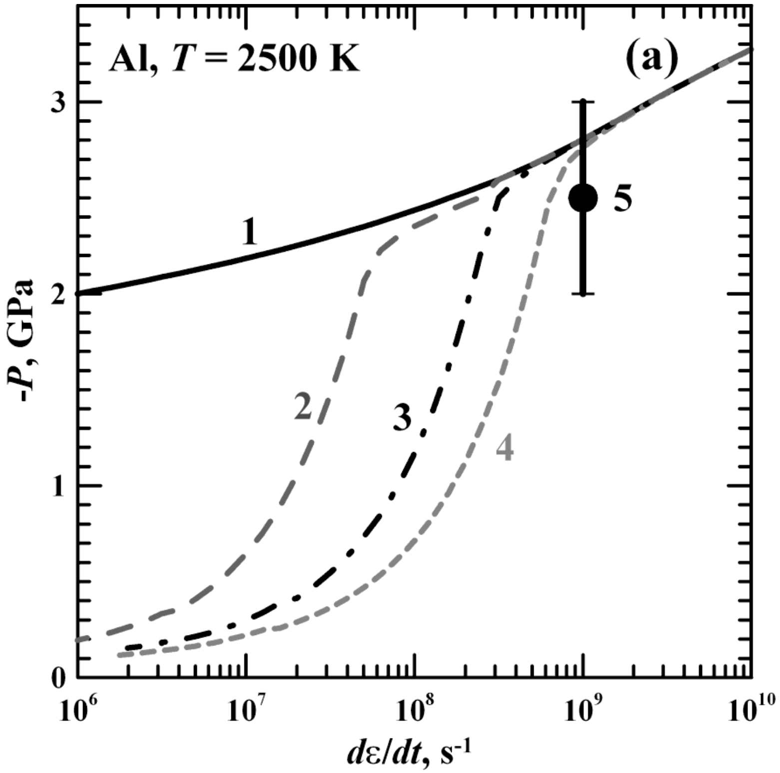
Soft and fusible inclusion

Mg inclusions (2.4 at.%) in Al melt (1100 K)

System	Mg	Al+Mg				Al
Preparation time (ps)	-	30	140	240	1200	-
Strength (GPa)	0.85	1.75	2.96	3.38	3.95	4.28

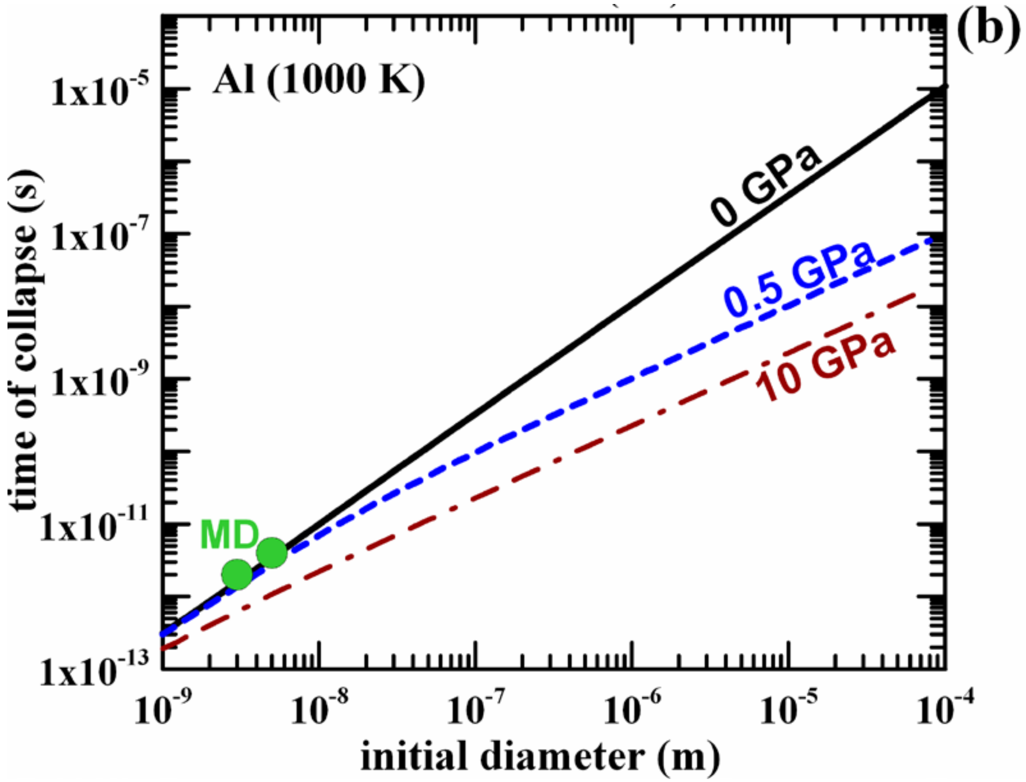


Initial pores



$$dN = \frac{2n_0}{\sqrt{\pi}R_0}\exp\left[-\left(\frac{R}{R_0}\right)^2\right]dR$$

Mayer A.E., Mayer P.N. // JETP Letters. (2015)
http://dx.doi.org/10.1134/S0021364015140088



Solid metals

Solid metal: continuum model based on molecular dynamics

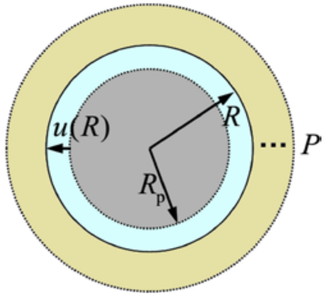
Growth of voids

growth rate of void is determined by the plastic deformation by means of the dislocations motion in the void vicinity

$$\left(\dot{R}\right)_p = R\left[\left(2\sigma_\tau^{\max}/Y\right)^{1/3} - 1\right]\left(bV_D\rho_D/\sqrt{6}\right)$$

Krasnikov V.S., Mayer A.E. // Int. J. Plast. (2015)
http://dx.doi.org/10.1016/j.ijplas.2015.06.007

$$\sigma_\tau^{\max} = \frac{G}{K}P - 3G\frac{\gamma/R + P\left(G/K + 1/2\right)}{2G - \gamma/R}$$



G shear modulus $K = \rho c^2$ bulk modulus

γ surface tension Y static yield strength

$$V_D = \left(b/B\right)\left[\sigma_\tau^{\max} - Y/2\right]\left[1 - \left(V_D/c_t\right)^2\right]^{3/2}$$

c_t transverse sound speed

$$\frac{d\rho_D^v}{dt} = \frac{0.1}{\varepsilon_D}\left(b\sigma_\tau^{\max}V_D\right)\left(\rho_D^a + \rho_D^v\right) - b\rho_D^v\left(\rho_D^a + \rho_D^v\right)V_D + \frac{\pi c_t}{2}n\left(\frac{4\pi R^2 b}{a_c^3}\right)\exp\left(-\frac{\pi\varepsilon_s a_c}{2k_B T}\right),$$

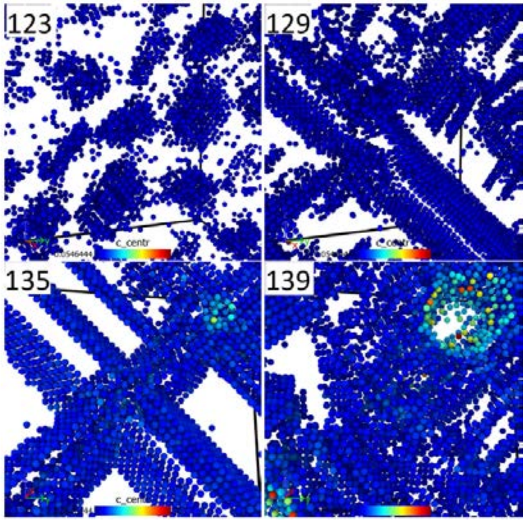
ρ_D^a macroscopic dislocation density ρ_D^v dislocation density in the void vicinity

$Y = Y_0 + 0.5Gb\sqrt{\rho_D}$ deformation hardening

Nucleation of voids

void nuclei arise within the areas of intersection of the stacking fault planes, which can exist initially or be formed in the course of deformation before the fracture beginning

Krasnikov V.S., Mayer A.E. // J. Phys.: Conf. Ser. (2015)
http://dx.doi.org/10.1088/1742-6596/653/1/012094



$$W_c = \frac{16\pi\gamma^3}{3k_B T P^2}\chi$$ work of formation of a critical pore

χ reduction factor

$$(\dot{n})_1 = \frac{c}{a^4}\exp(-W_c)\cdot(1-\alpha)$$ nucleation rate

critical voids with radius $R_c = 2\gamma/(-P)$

Initially existing voids

Pogorelko V.V., Mayer A.E. // Mater. Sci. Eng.: A (2015)
http://dx.doi.org/10.1016/j.msea.2015.07.009

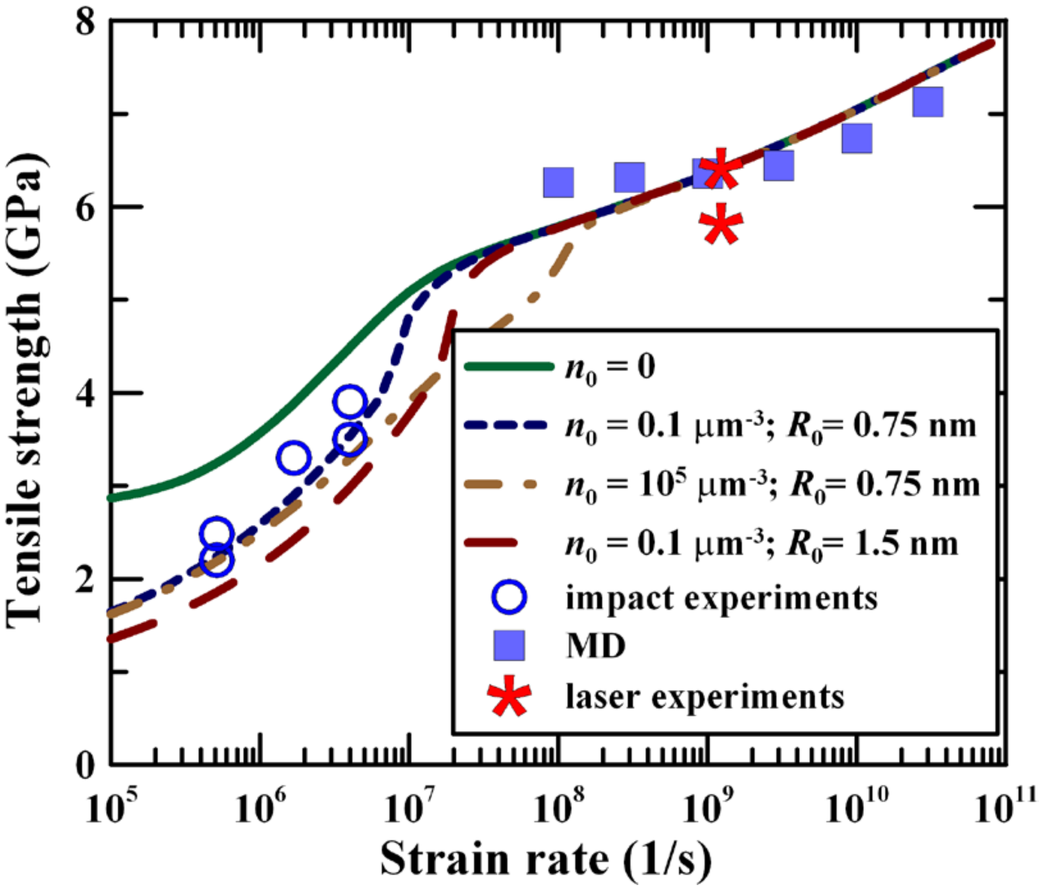
suppose an exponential distribution of voids over their surface area

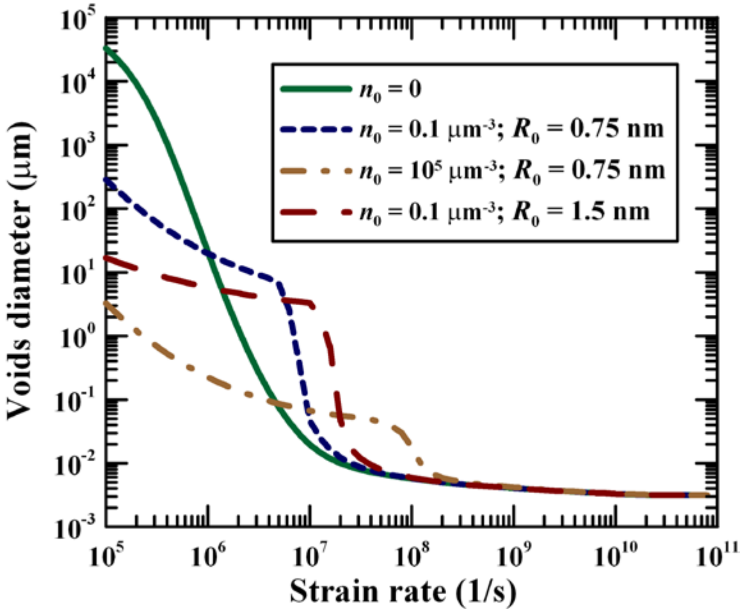
$$(\dot{n})_2 = \frac{2n_0}{\sqrt{\pi}R_0}\exp\left(-\left[\frac{R_c}{R_0}\right]^2\right)\left|\frac{dR_c}{dt}\right|\theta\left(-\frac{dR_c}{dt}\right)$$ additional rate of "nucleation" of the active voids

n_0 total concentration of the initial voids

$R_0/(2\pi^{1/2})$ average radius

Influence of model parameters





impact experiments – Kanel G.I., Razorenov S.V., Baumung K., Singer J. // J. Appl. Phys. (2001)
laser experiments – Ashitkov S.I., Agranat M.B., Kanel G.I., Komarov P.S., Fortov V.E.// JETP Lett. (2010)
MD – Pogorelko V.V., Mayer A.E. // Mater. Sci. Eng.: A (2015)

Influence of impurities

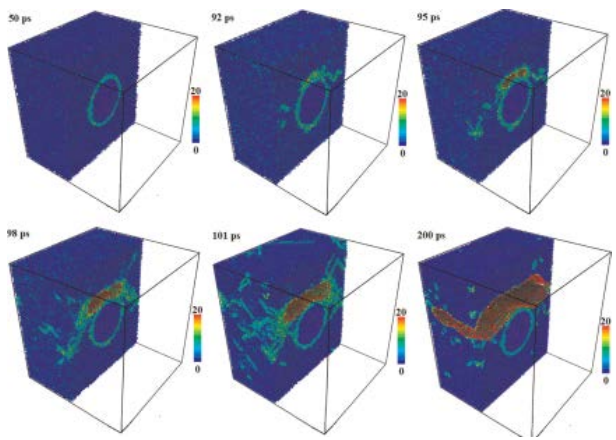
SOLID METAL

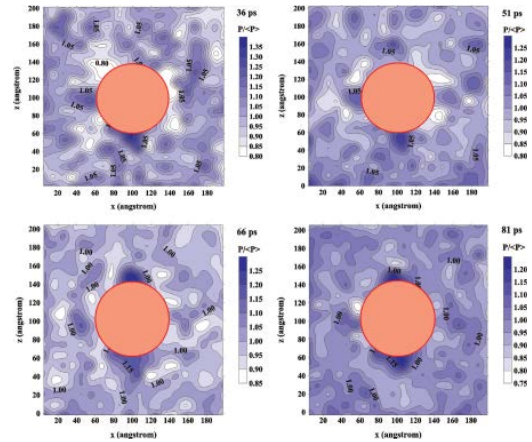
Inclusions can make metal weaker by different ways:

A) stress concentration in vicinity of strong and stiff inclusions (Cu or Ti in Al);

B) nucleation of voids inside inclusions made of a softer material compared with the matrix (Mg in Al);

C) nucleation of voids on the interface-for materials with close values of elastic and strength properties (Ni in Fe).





Pogorelko V.V., Mayer A.E. // Mater. Sci. Eng.: A (2015) http://dx.doi.org/10.1016/j.msea.2015.07.009

Pogorelko V.V., Mayer A.E. // Mater. Sci. Eng.: A (2016) http://dx.doi.org/10.1016/j.msea.2016.03.053

$$\alpha = \frac{4\pi}{3} R^3 n + \frac{4\pi}{3} R_1^3 n_1$$

Areas of stress concentration

All equations for R_1, n_1 are the same as for R, n with the following replacements

$P \to P_1 = K\,P$ $\quad$ $K > 1$ stress concentration factor (MD)

$(1-\alpha) \to (1-\alpha)(0.1\alpha_c)$ $\quad$ α_c volume fraction of inclusions

Weak inclusions

For R_1, n_1 we have following replacements

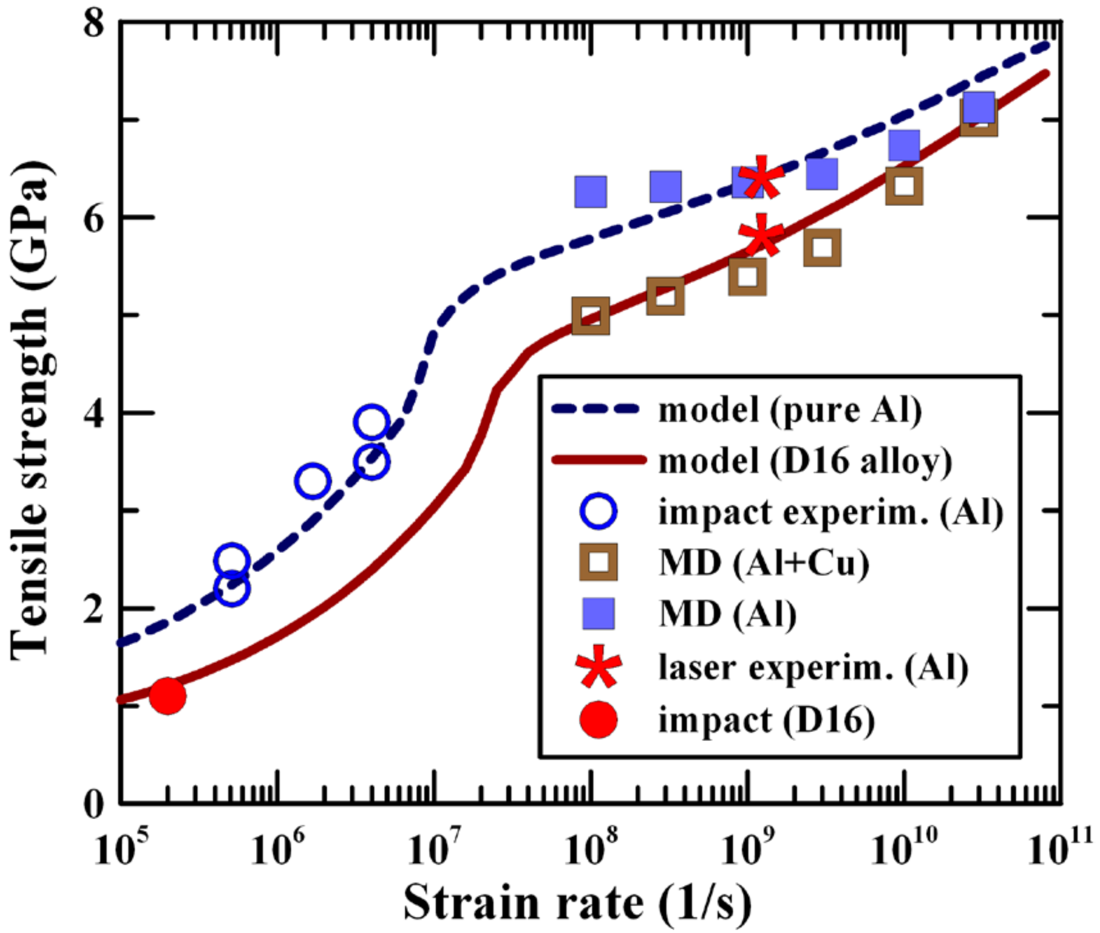
$$(\gamma, \chi, P) \to (\gamma_1, \chi_1, P_1) = \begin{cases} (\gamma_{incl}, \chi_{incl}, M\,P), & R \le R_{incl} \\ (\gamma, \chi, P), & R > R_{incl} \end{cases}$$

$M < 1$ ratio of pressure inside inclusion and average one (MD)

Weak boundary

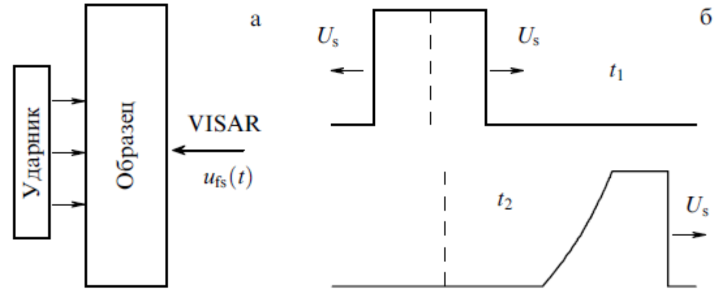
Replacements only for n_1 (nucleation and activation of pores) $\quad \chi \to \chi_1$

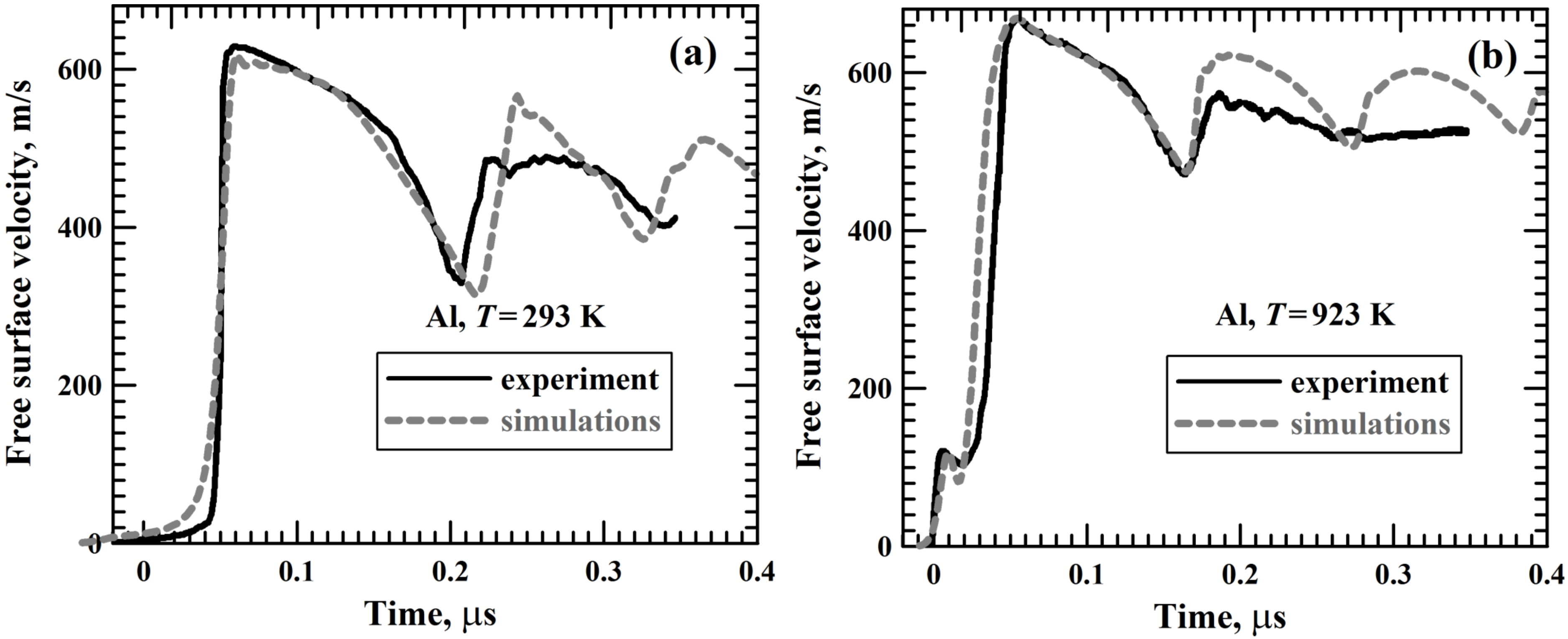
Al and D16 alloy: strength



impact exper. (Al) – Kanel G.I., Razorenov S.V., Baumung K., Singer J. // J. Appl. Phys. (2001)
laser experim. (Al) – Ashitkov S.I., Agranat M.B., Kanel G.I., Komarov P.S., Fortov V.E.// JETP Lett. (2010)
Impact D16 – Garkushin G.V., Razorenov S.V., Kanel G.I. // Phys. Solid State (2008)
MD – Pogorelko V.V., Mayer A.E. // Mater. Sci. Eng.: A (2015)

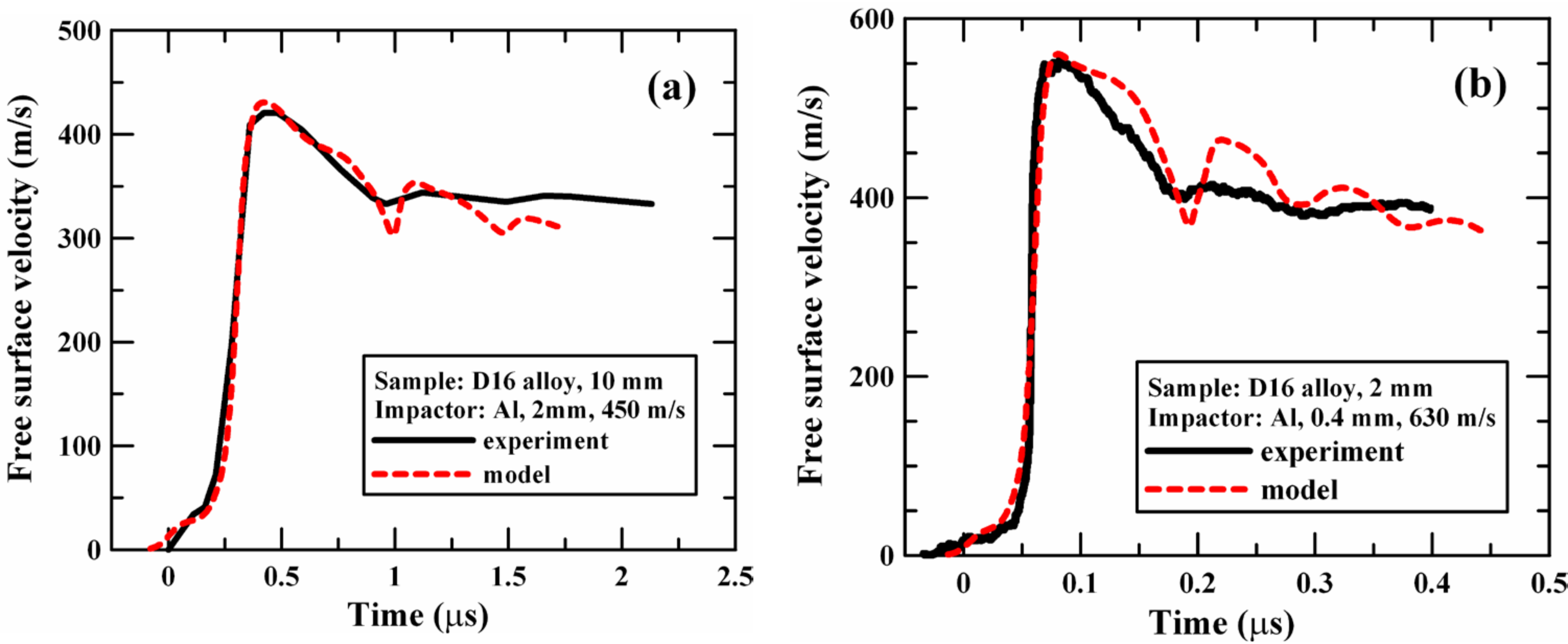
Rear surface velocity histories





Experimentl data: **[Kanel G.I., Razorenov S.V., Baumung K., Singer J. // J. Appl. Phys. (2001)]**

D16 alloy: rear surface velocity histories for high-velocity impact



experimental data:

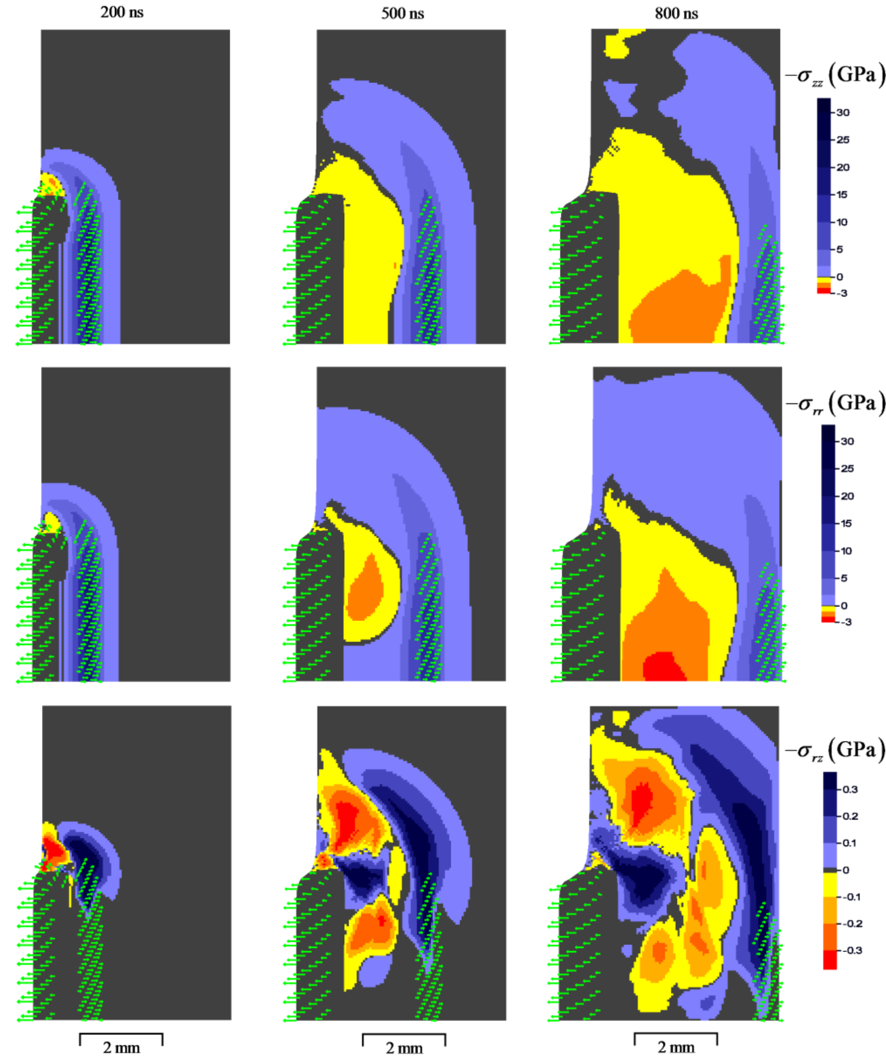
(a) – **[Kanel, Razorenov, Utkin, Baumung (1996) Experimental profiles of shock waves]**

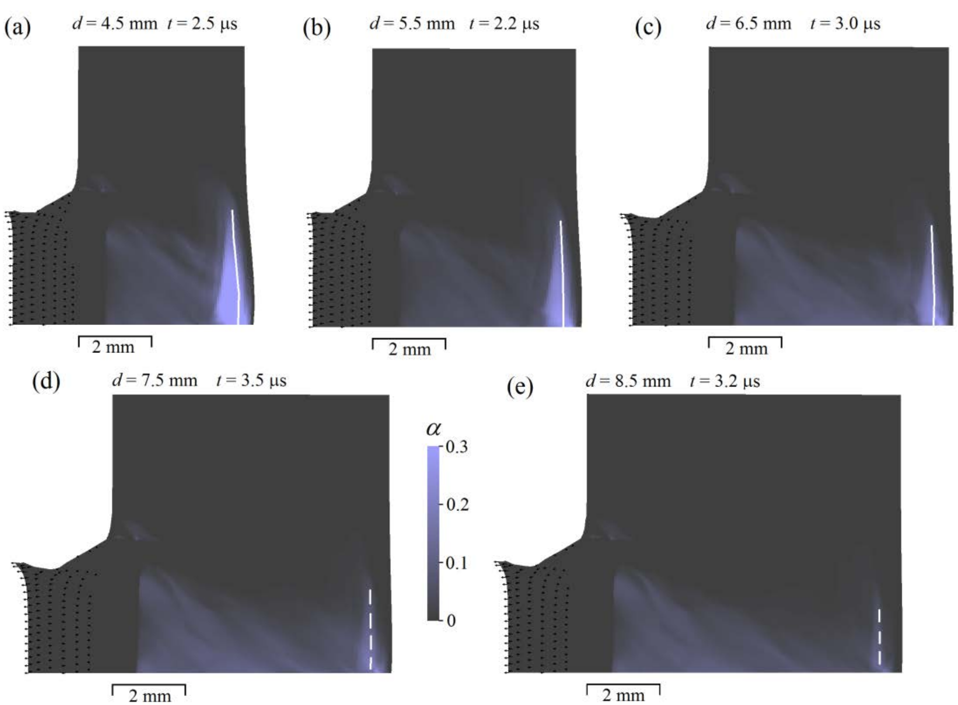
(b) – **[Garkushin, Razorenov, Kanel // Phys. Solid State (2008)]**

High-current electron irradiation of stainless steel

SINUS-7 electron accelerator (Tomsk, Russia, Institute of High Current Electronics SB RAS)

The maximal energy of electrons is 1.35 MeV, the pulse duration is 45 ns, the maximal power density is 34 GW/cm^2, and the incident energy density is 1.2 kJ/cm^2.





Gnyusov S.F., Rotshtein V.P., Mayer A.E., Rostov V.V., Gunin A.V., Khishchenko K.V., Levashov P.R. // Int. J. Fracture (2016) http://dx.doi.org/10.1007/s10704-016-0088-8

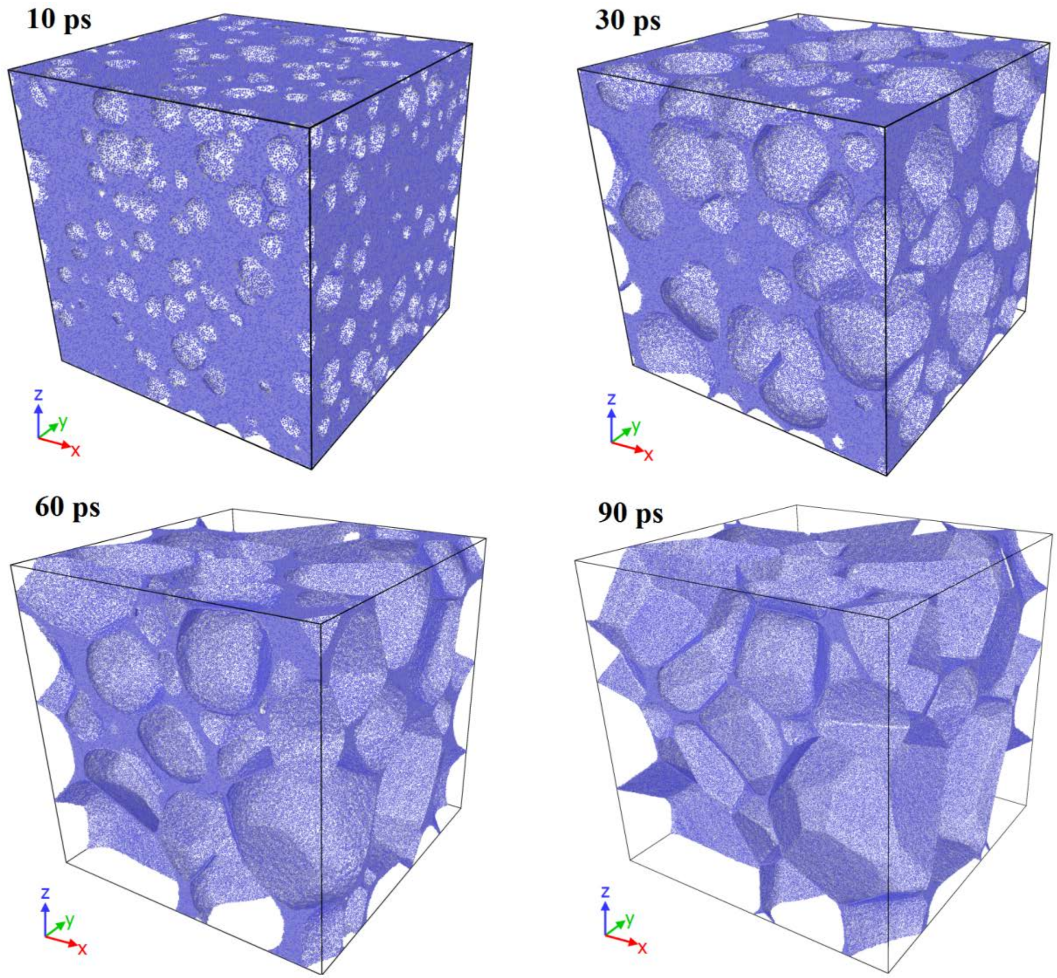
Late stages of fracture

Late stages of fracture of metal melt

MD simulation (Al melt 30/ns, 1100K)

4 million atoms

0.3 **0.9**

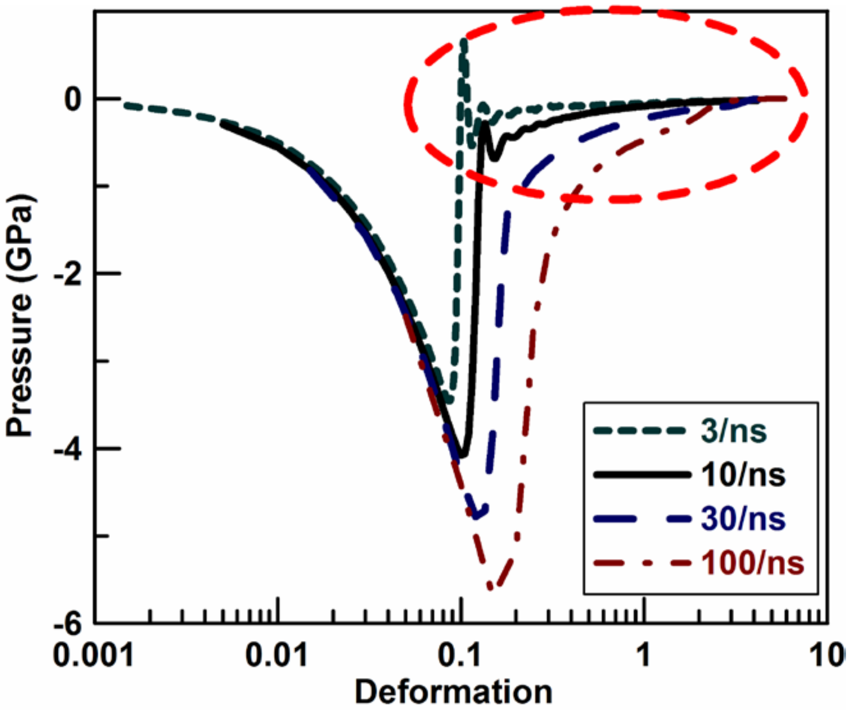


1.8 **2.7**

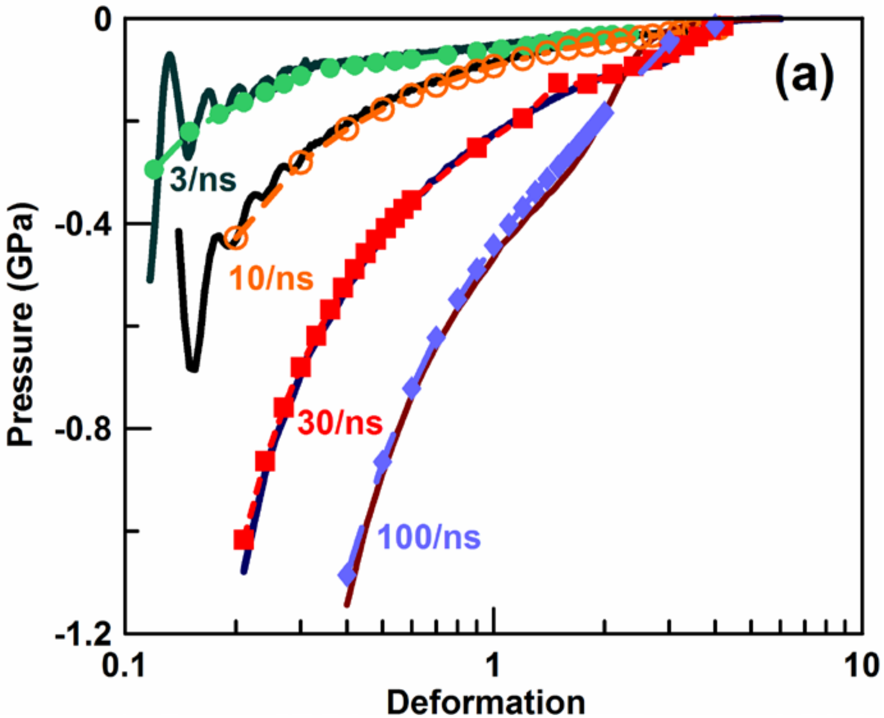
***V* / *V*₀ = 15**

Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016) http://dx.doi.org/10.1063/1.4959819

Pressure at the stage of foamed melt



$$P = -\frac{2\sigma}{R_p}$$



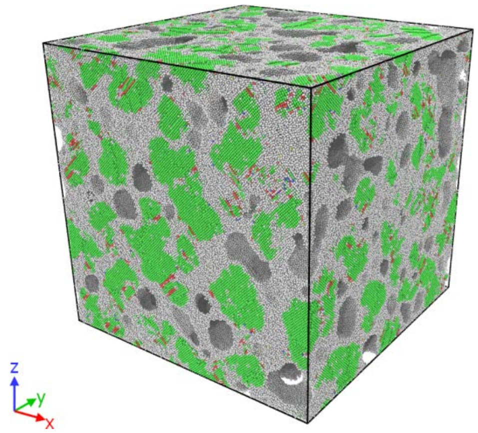
Al melt 30/ns, 1100K

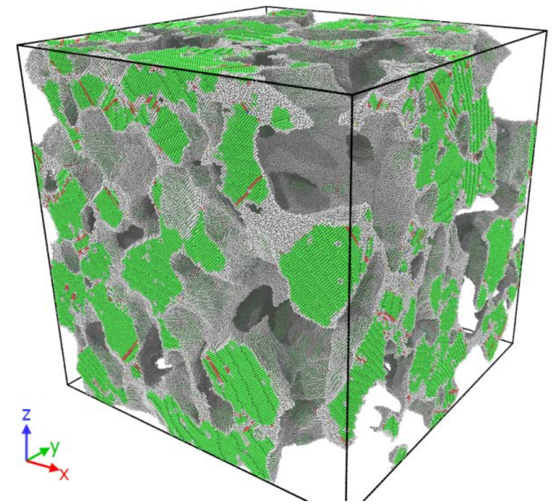
Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016) http://dx.doi.org/10.1063/1.4959819

Late stages of solid metal fracture

Al, 300K, true strain rate is 10/ns, 4 million atoms

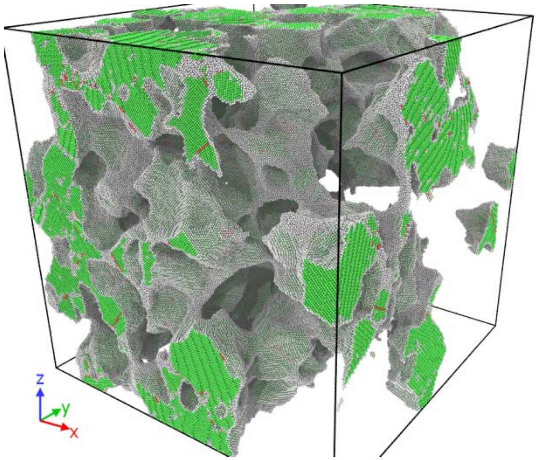
30 ps
V/V0=
1.35

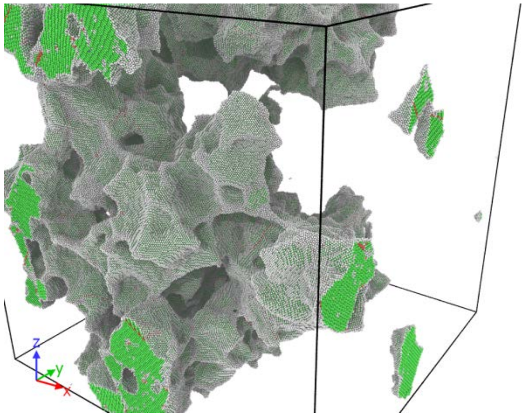




70 ps
V/V0=
2

100 ps
V/V0=
2.7





150 ps
V/V0=
4.5

Interatomic potential **[Mishin Y., Farkas D. , Mehl M.J., Papaconstantopoulos D.A. // Phys. Rev. B (1999)]**

Conclusions

- The developed approaches is aimed to bridge the atomistic-scale simulations with macroscopic scale.
- The material defects are incorporated into the continuum mechanics model through their observable characteristics, such as radii and concentrations.
- MD simulations are useful for both the determination of the defects evolution equations and the parameter determination.
- The complete fracture corresponds to the void volume fracture more than 0.8 from the system volume.
- Work required for fragmentation exceeds several times the work on reaching the maximal tensile strength

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