FORMATION OF FOAMED STRUCTURE IN ALUMINUM AND IRON MELTS AT HIGH-RATE TENSION

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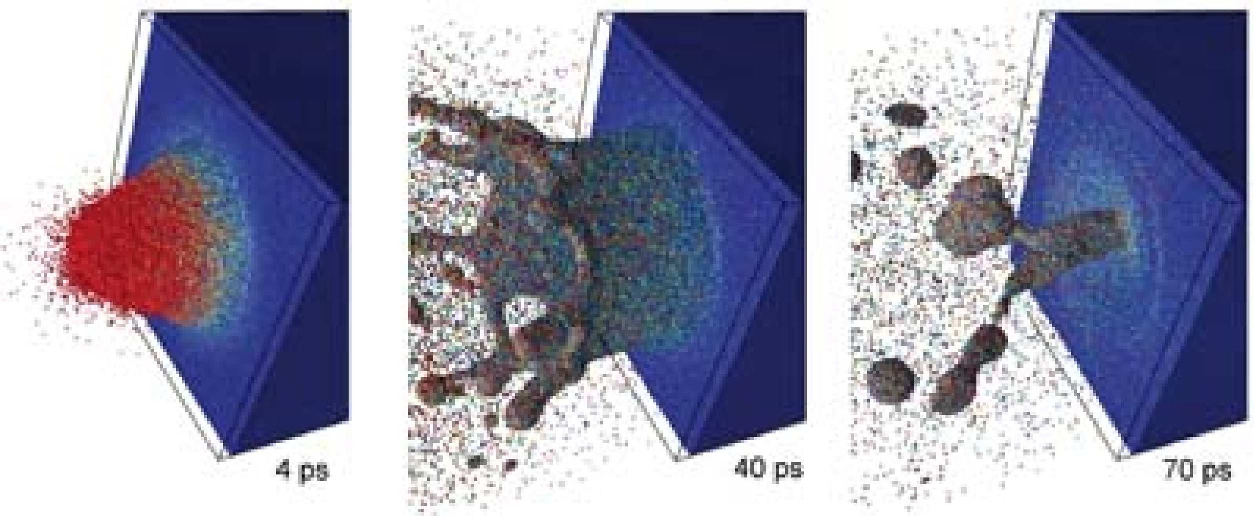
March 22, 2017

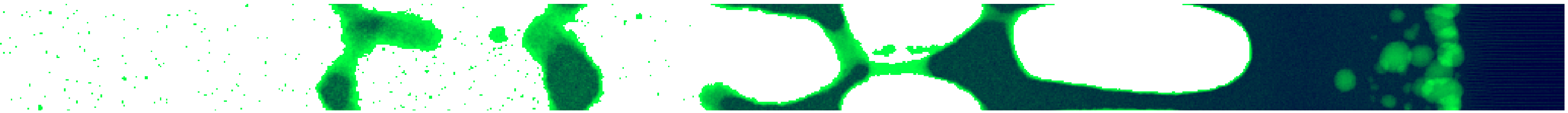
Problem statement

Evolution of metal surface after powerful 100 fs laser irradiation (MD simulations)



[Roth J., Sonntag S., Karlin J., and Trebin H.-R. // InSiDe (Innovatives Supercomputing in Deutschland) (2012)]

Irradiation of tantalum film by powerful ultra-short laser pulse (MD simulations)



[Inogamov N.A., et al. // Contrib. Plasma Phys. (2013)]

High-rate tension of Al melt

LAMMPS [Plimpton S. // J. Comp. Phys. (1995) http://lammps.sandia.gov]
OVITO [Stukowski A. // Modell. Simul. Mater. Sci. Eng. (2010) http://www.ovito.org]
"Construct surface mesh" algorithm [Stukowski A. // JOM (2014)]

4 000 000 atoms

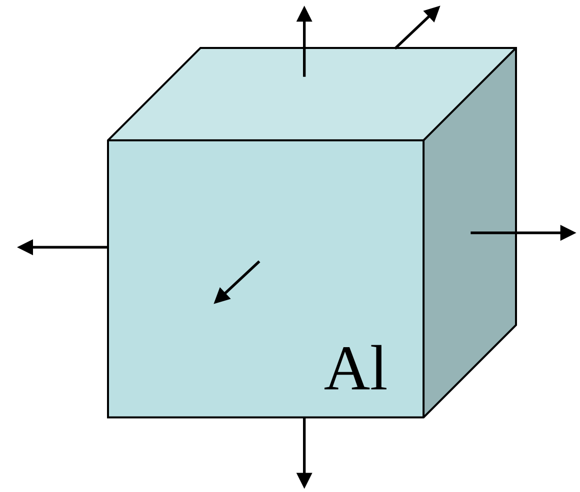
Initial temperature is 2500 K to ensure melting

Uniform tension at constant temperature of 1100 K

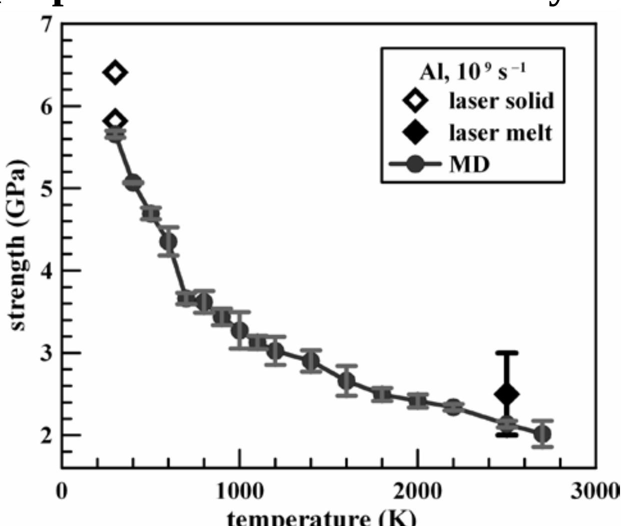
Strain rates (true) are 3, 10, 30 and 100/ns

$$\varepsilon = \ln\left(V / V_0\right)$$

Degree of deformation is from 2.5 to 10



Interatomic potential for Al
[Zope R.R. and Mishin Y. // Phys. Rev. B. 68, 024102 (2003)]

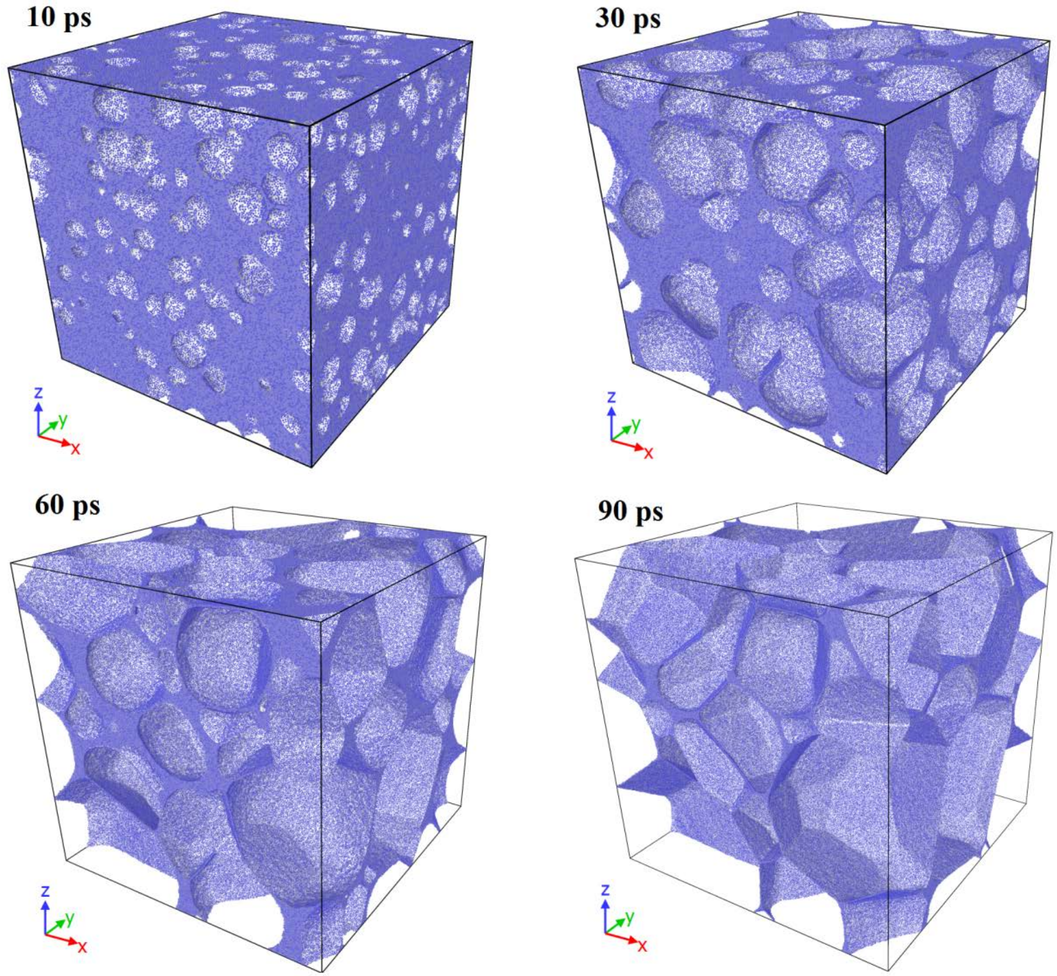


laser solid [Ashitkov S.I., Agranat M.B., Kanel G.I., Komarov P.S., Fortov V.E. // JETP Lett. (2010)]
laser melt [Agranat M.B., Anisimov S.I., Ashitkov S.I., Zhakhovskii V.V., Inogamov N.A., Komarov P.S., Ovchinnikov A.V., Fortov V.E., Khokhlov V.A., Shepelev V.V. // JETP Lett. (2010)]
MD [Mayer A.E., Mayer P.N. // Comp. Mat. Sci. (2016)]

Late stages of high-rate tension of Al melt: cavities and foamed melt

0.3

0.9



1.8

2.7

$V / V_0 = 15$

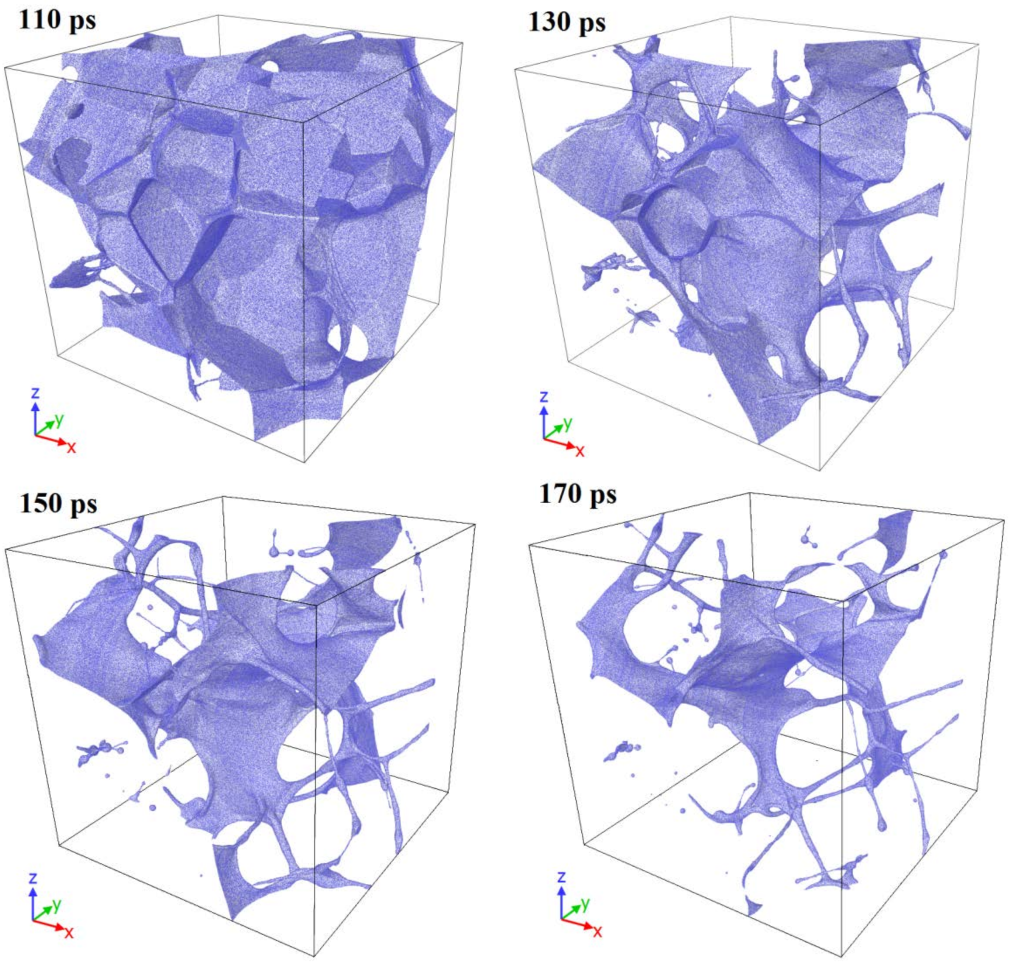
Strain rate is 30/ns, temperature is 1100K

[Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016)]

Late stages of high-rate tension of Al melt: breaking of walls and decay on jets

3.3

3.9



4.5

5.1

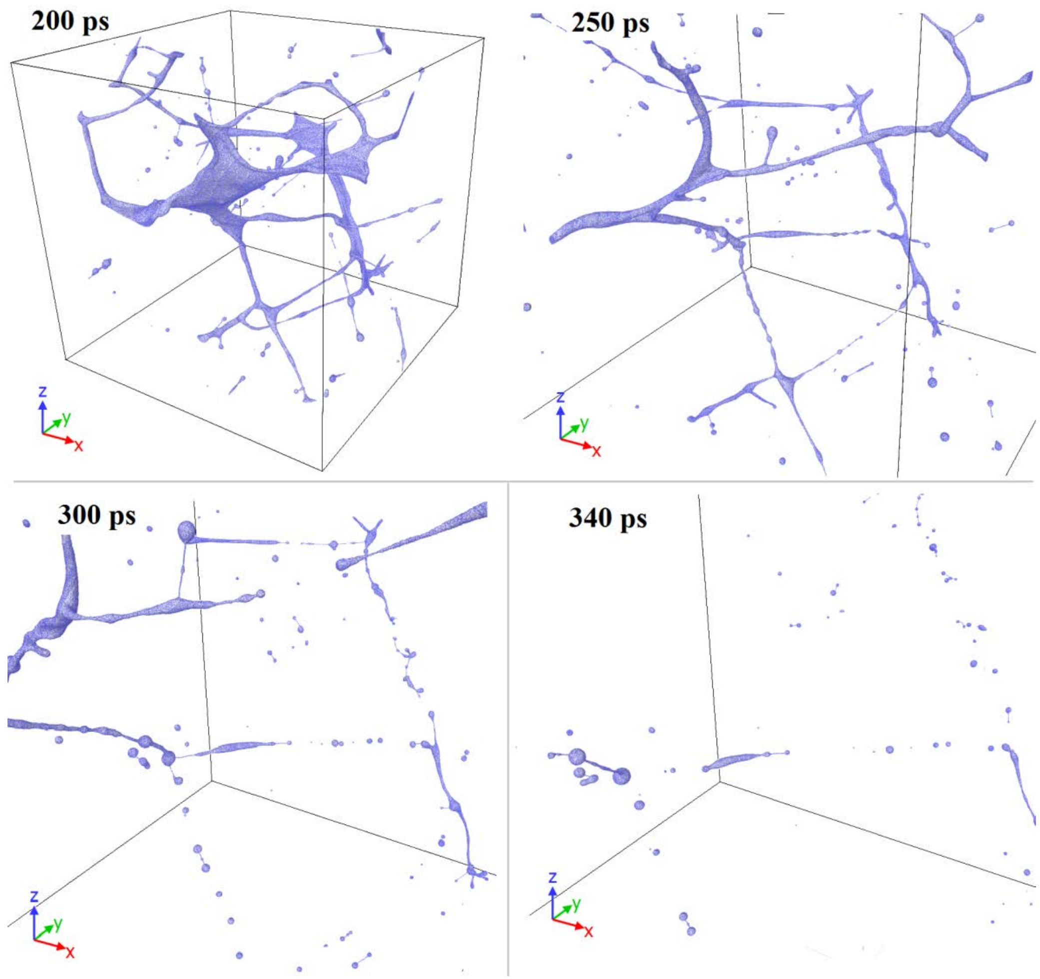
$V / V_0 = 164$

Strain rate is 30/ns, temperature is 1100K

[Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016)]

Late stages of high-rate tension of Al melt: breaking of jets on droplets

6 7.5



9 10.2

$V / V_0 = 2690$

Strain rate is 30/ns, temperature is 1100K

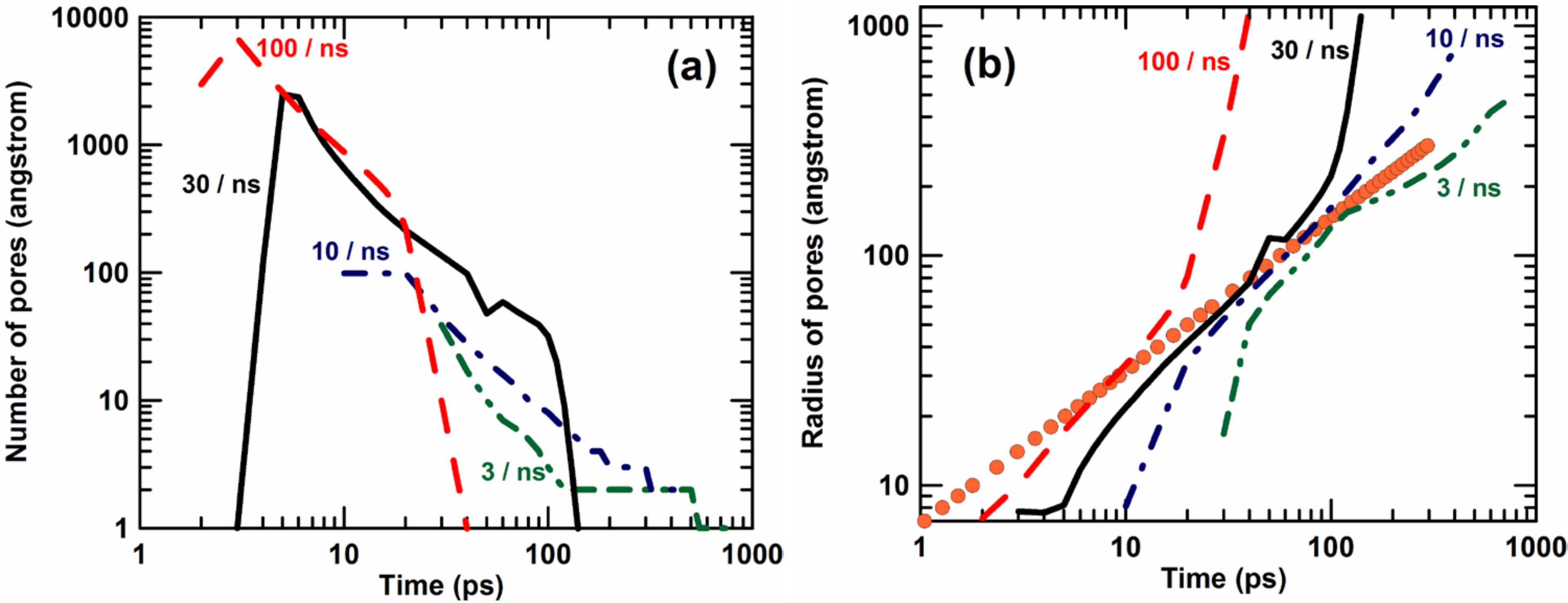
[Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016)]

Evolution of pores in Al melt at tension

Estimations: $R_p = 3\frac{(V-V_S)}{S}$ $N_p = \frac{1}{36\pi}\frac{S^3}{(V-V_S)^2}$

S is surface area

V is total volume V_S is liquid volume



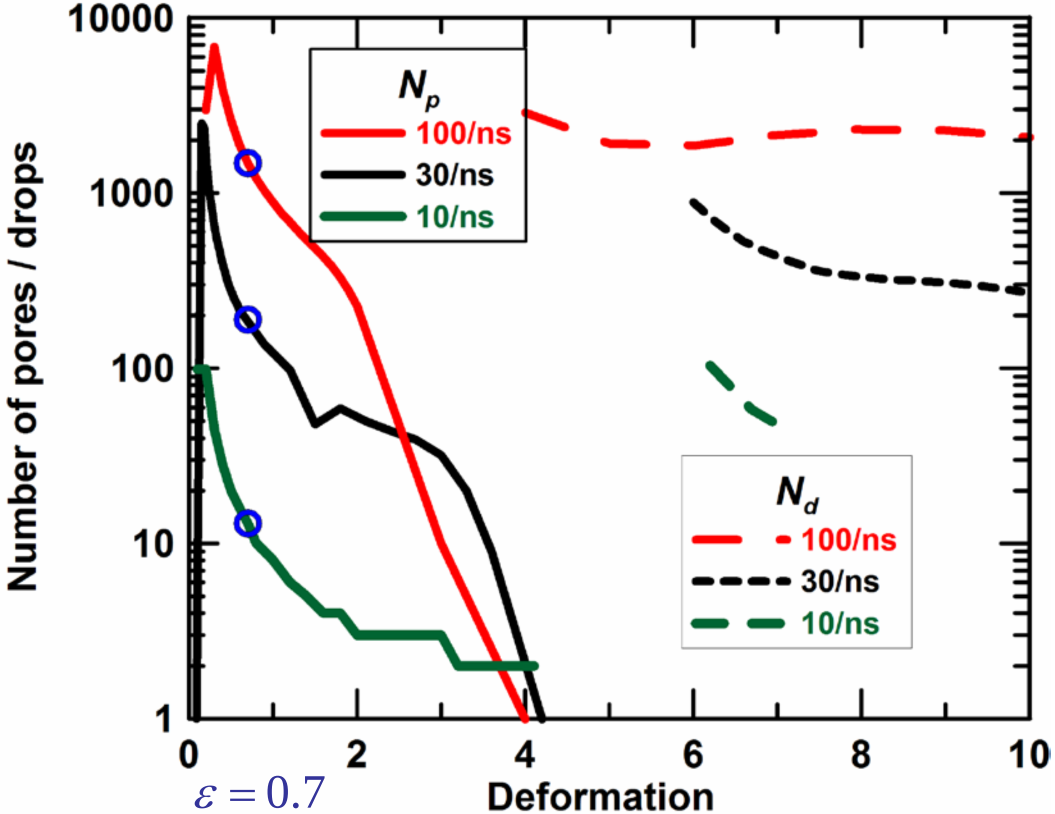
$\tau = \sqrt{\frac{R_p^3\rho}{\sigma}}$ typical time of a pore radius variation under the action of surface tension

$$\Rightarrow R_p = \frac{t^{2/3}\sigma^{1/3}}{\rho^{1/3}}$$

[Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016)]

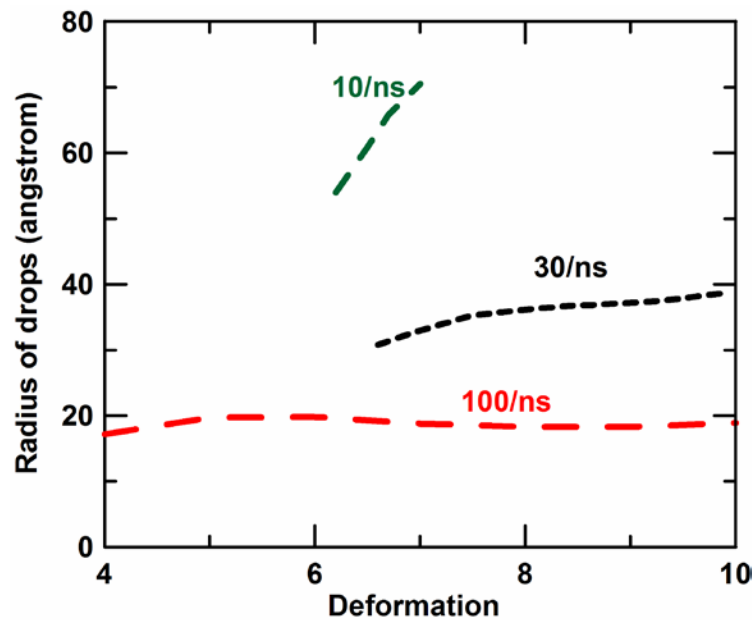
Characteristics of droplets

Correlation between numbers of pores and droplets



$\varepsilon = 0.7$

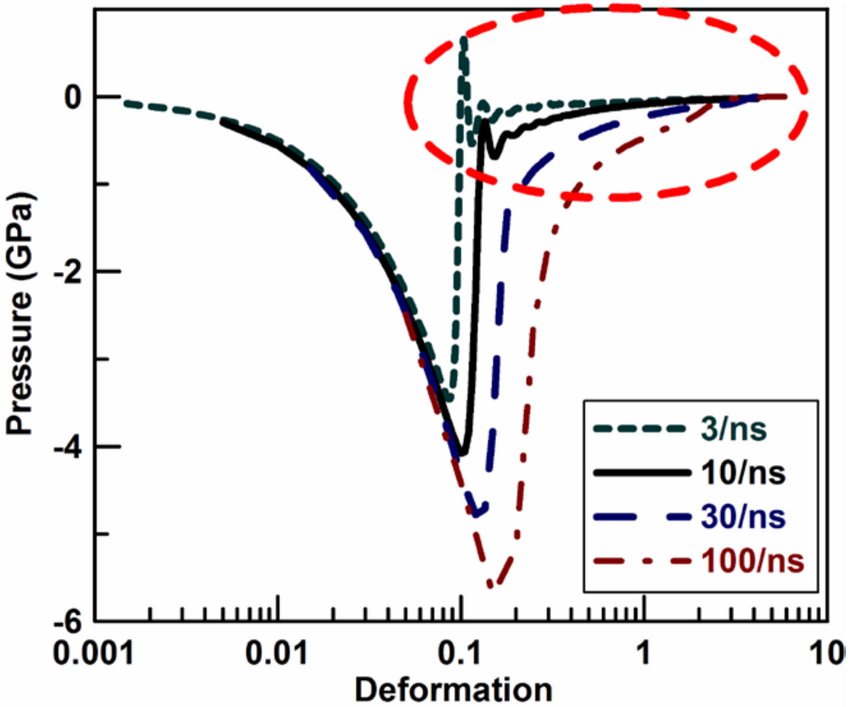
$(V/V_0 \approx 2)$



[Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016)]

Pressure at the stage of foamed Al melt

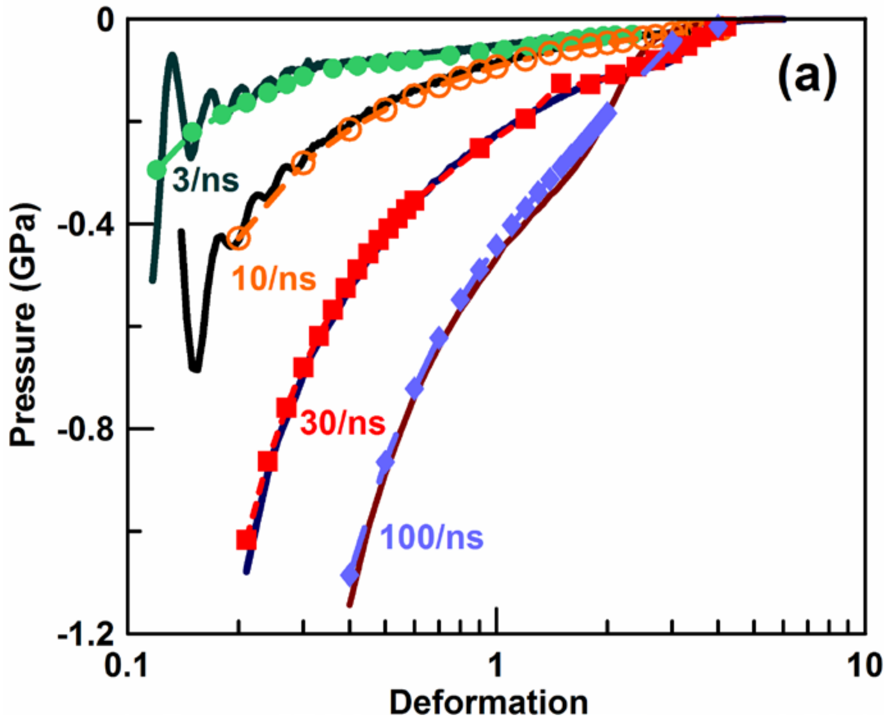
temperature is 1100K



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

$$\sigma = 0.743\ \mathrm{J/m^2}$$

$$\sigma_{\mathrm{MD}} = 0.57\ \mathrm{J/m^2}$$

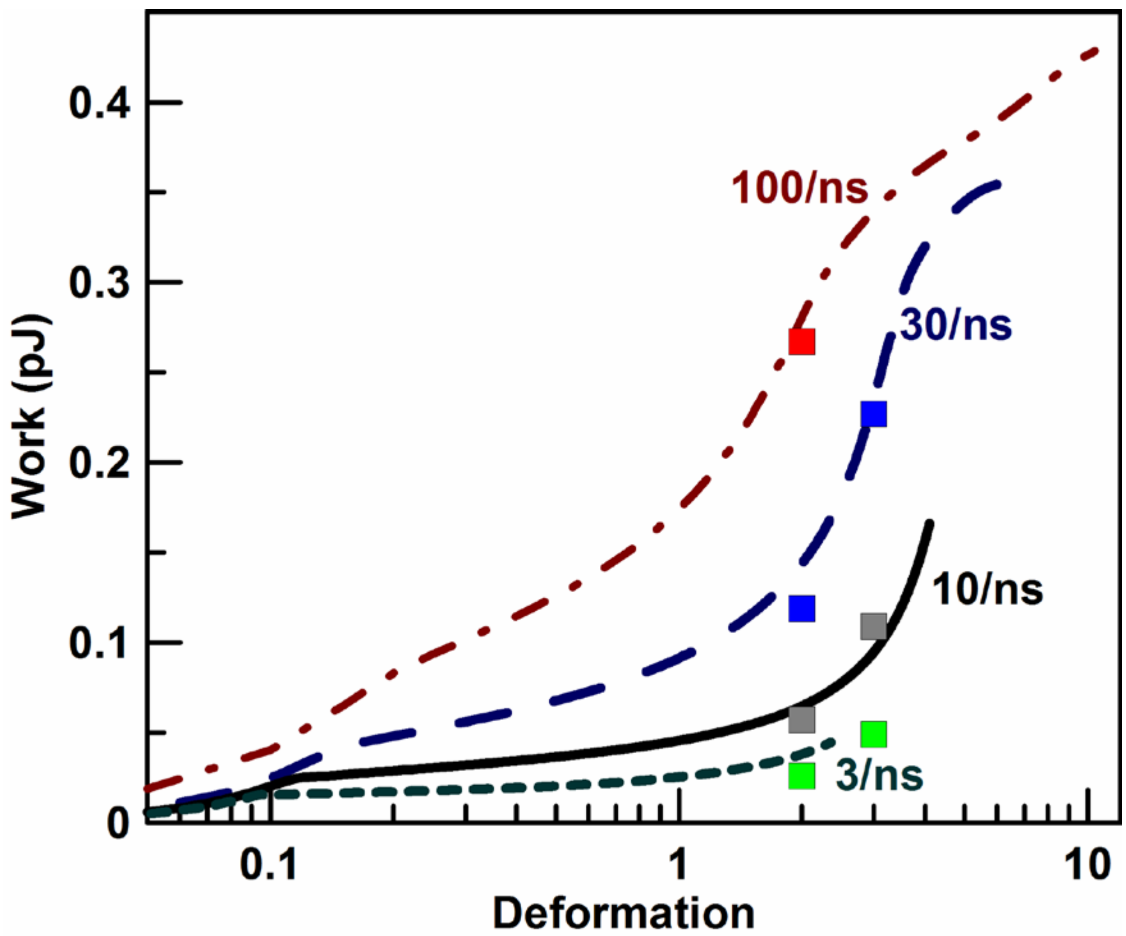


$$P = -2\sigma\left\langle\frac{1}{R}\right\rangle \qquad \frac{1}{R_p} = \frac{\langle R^2\rangle}{\langle R^3\rangle}$$

=> investigation of the void size distribution is required

[Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016)]

Work spent on deformation of MD system



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

$$R_p = \frac{t^{2/3}\sigma^{1/3}}{\rho^{1/3}}$$

$$W(\varepsilon) = -V_0 \int_0^{\varepsilon} P(\varepsilon') \times \exp(\varepsilon')\, d\varepsilon'$$

$$\boxed{W = 2V_0 \left(\rho^{1/3}\sigma^{2/3}\dot{\varepsilon}^{2/3}\right) \int_0^{\varepsilon} (\varepsilon')^{-2/3} \times \exp(\varepsilon')\, d\varepsilon'}$$

[Mayer P.N., Mayer A.E. // J. Appl. Phys. (2016)]

High-rate tension of Fe melt

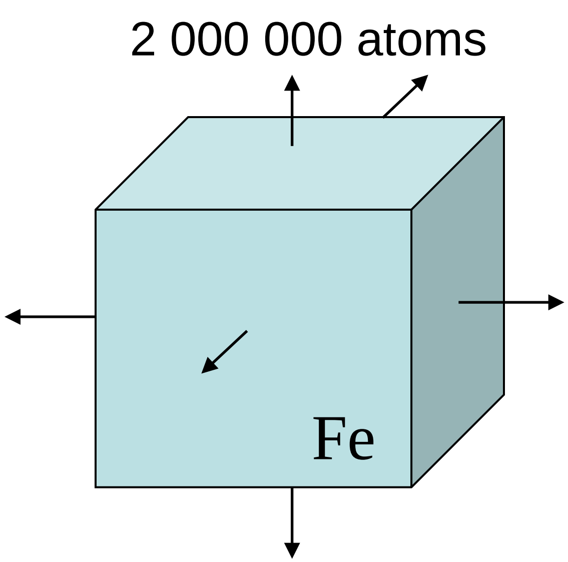
LAMMPS [Plimpton S. // J. Comp. Phys. (1995) http://lammps.sandia.gov]
OVITO [Stukowski A. // Modell. Simul. Mater. Sci. Eng. (2010) http://www.ovito.org]
"Construct surface mesh" algorithm [Stukowski A. // JOM (2014)]

Initial temperature is 3000 K to ensure melting

Uniform tension at constant temperature of 2000 K

Strain rates (true) 10, 30 and 100/ns

Maximal degree of deformation is about 11



Interatomic potential for Fe
[Zhou, X.W., Johnson, R.A., Wadley, H.N.G. // Phys. Rev. B. (2004)]

Tensile strength of Fe melt at the strain rate of (0.4-0.9)/ns and temperature of 3000 K:

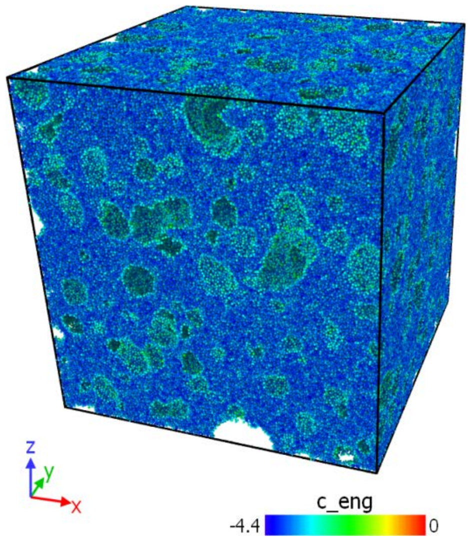
0.5-1.3 GPa according to the experimental data **[Struleva, E.V., Ashitkov, S.I., Komarov, P.S., Khishchenko, K.V., Agranat, M.B., // J. Phys.: Conf. Ser. (2016)]**

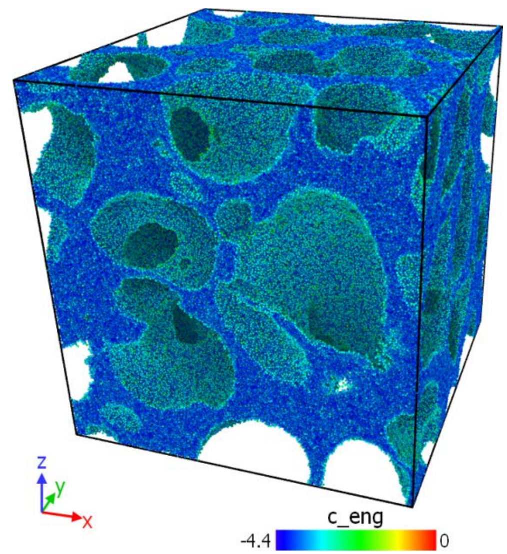
2 GPa according to MD simulations **[Mayer A.E., Mayer P.N. // J. Appl. Phys. (2015)]** with this potential

Nucleation, growth and consolidation of cavities in foamed Fe melt

temperature is 2000 K; strain rate is 30/ns

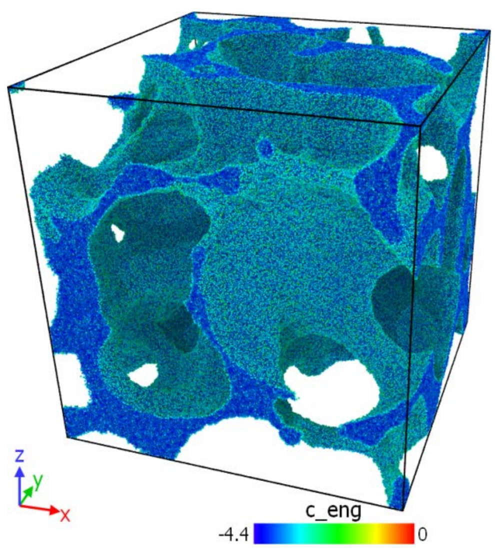
10 ps
ε = 0.3
$V/V0$ = 1.35

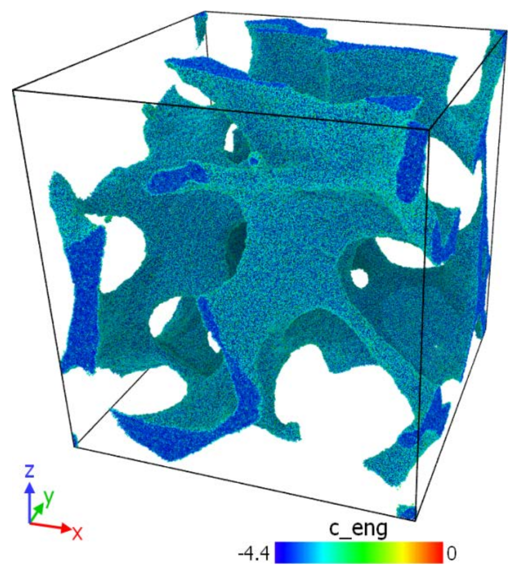




30 ps
ε = 0.9
$V/V0$ = 2.5

50 ps
ε = 1.5
$V/V0$ = 4.5



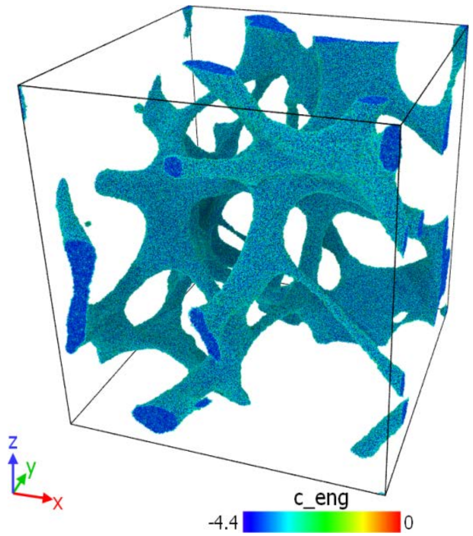


70 ps
ε =2.1
$V/V0$ = 8.2

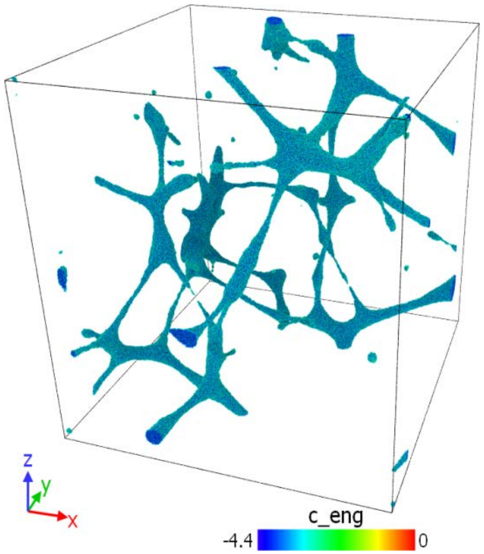
Destruction of foamed melt structure of jets and decay of jets on droplets

Fe melt, temperature is 2000 K; strain rate is 30/ns

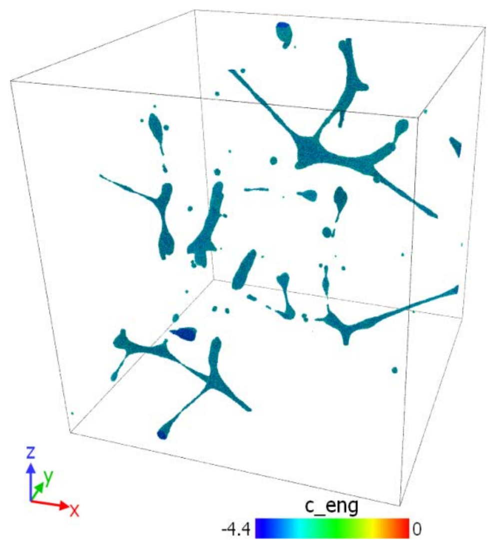
90 ps
ε = 2.7
***V*/*V*0 = 15**



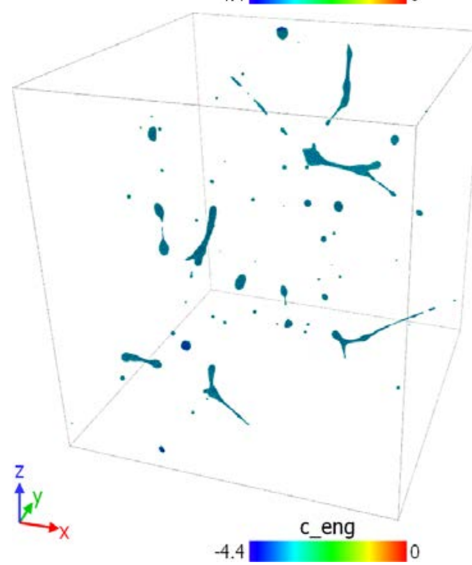
150 ps
ε = 4.5
***V*/*V*0 = 90**



200 ps
ε = 6
***V*/*V*0 = 400**



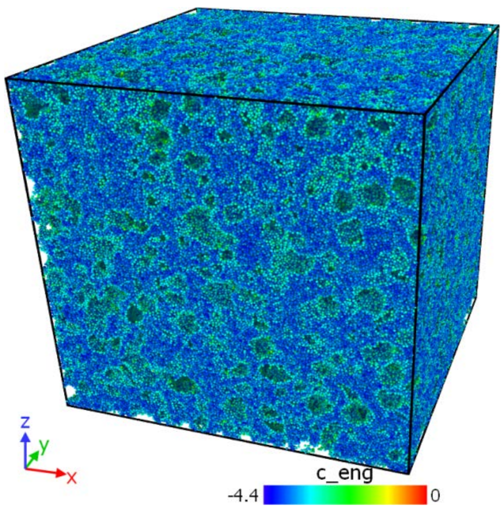
250 ps
ε =7.5
***V*/*V*0 = 1800**



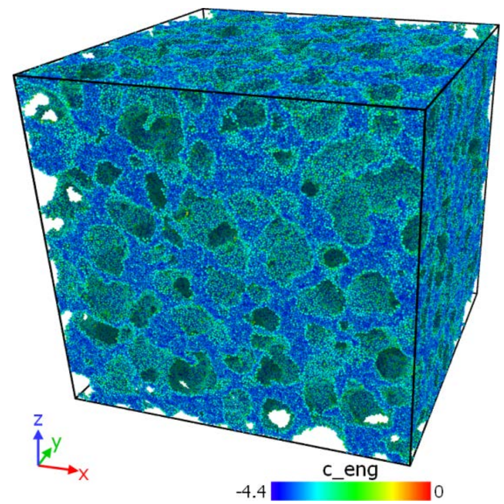
Nucleation, growth and consolidation of cavities in foamed Fe melt

temperature is 2000 K; strain rate is 100/ns

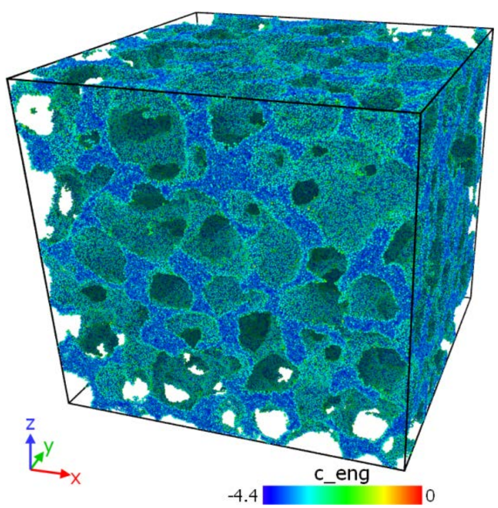
4 ps
ε = 0.4
***V*/*V*0 = 1.5**



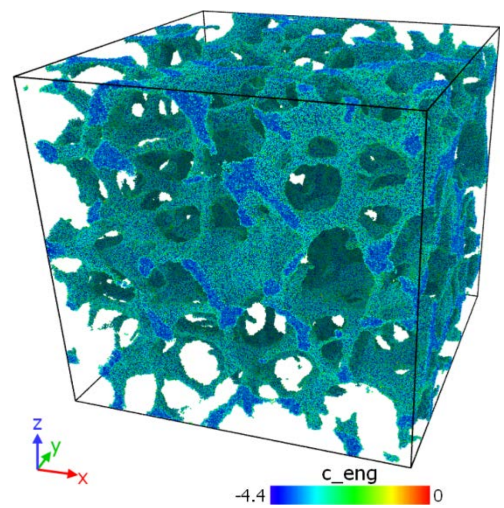
8 ps
ε = 0.8
***V*/*V*0 = 2.2**



12 ps
ε = 1.2
***V*/*V*0 = 3.3**



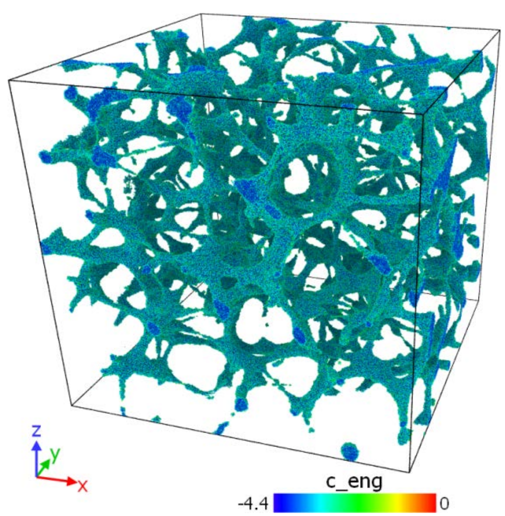
20 ps
ε =2
***V*/*V*0 = 7.4**

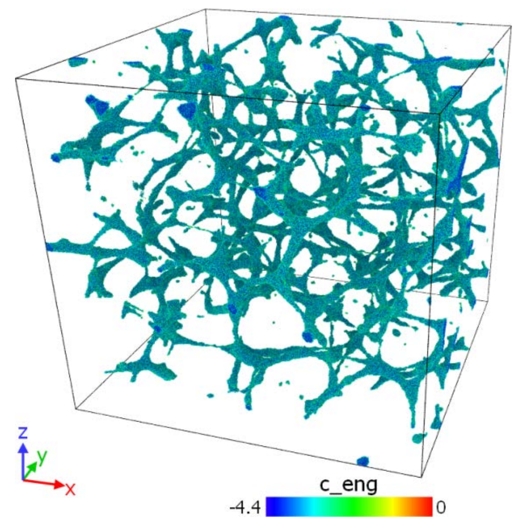


Destruction of foamed melt structure of jets and decay of jets on droplets

Fe melt, temperature is 2000 K; strain rate is 100/ns

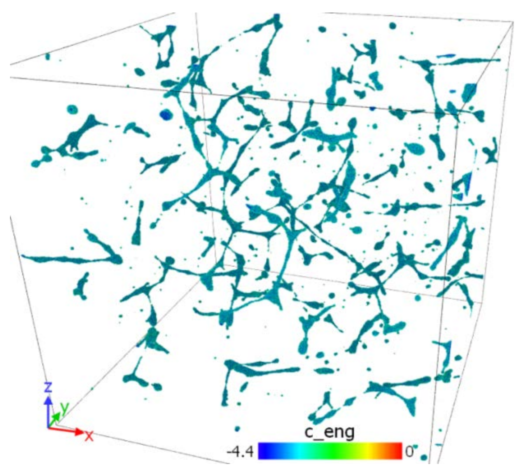
30 ps
$\varepsilon = 3$
$V/V0 = 20$

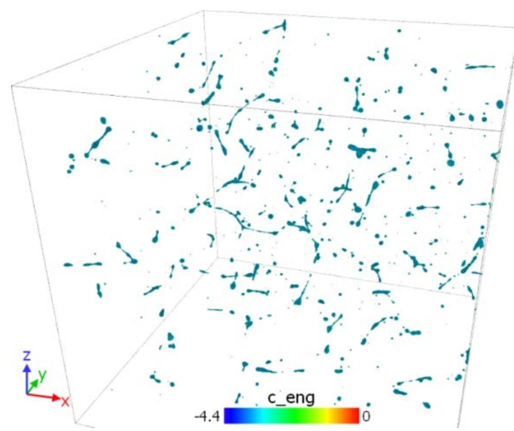




40 ps
$\varepsilon = 4$
$V/V0 = 55$

60 ps
$\varepsilon = 6$
$V/V0 = 400$

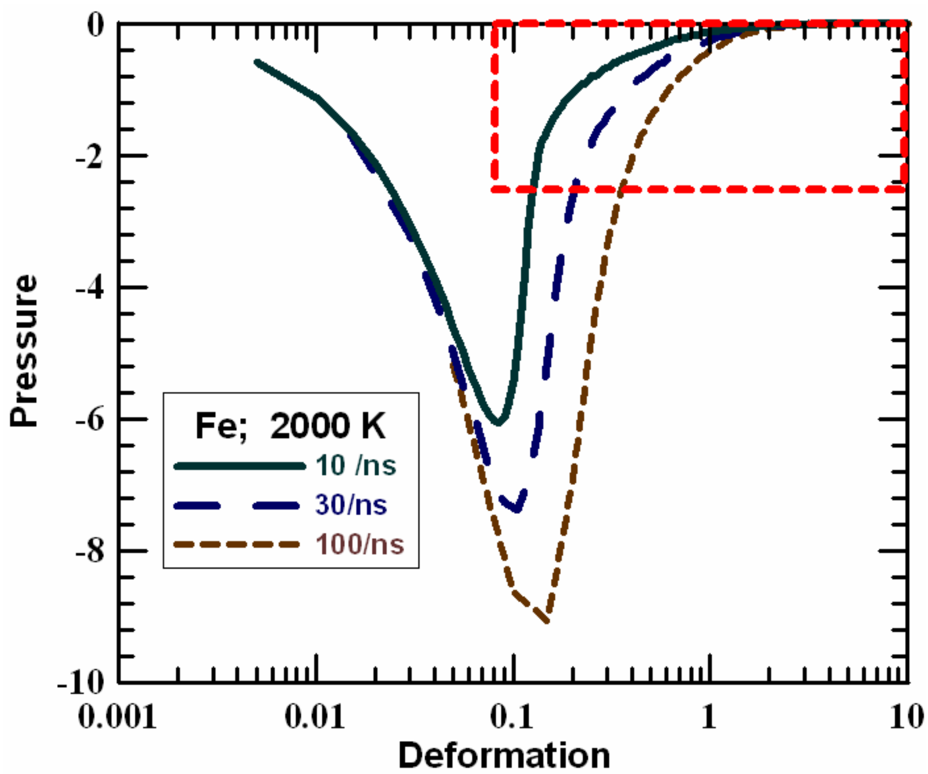




80 ps
$\varepsilon = 8$
$V/V0 = 3000$

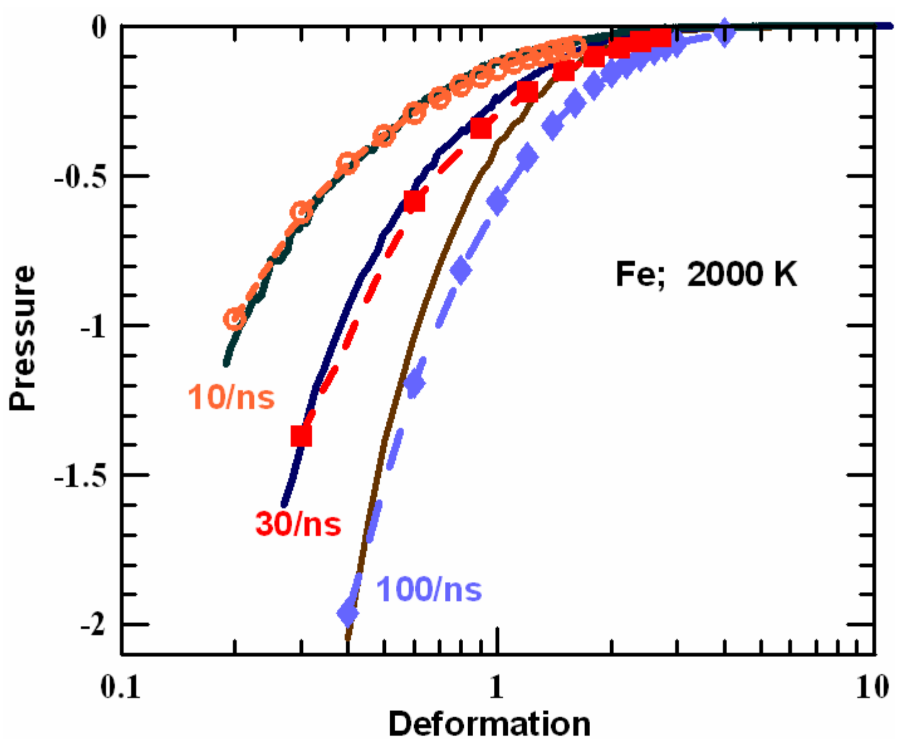
Pressure at the stage of foamed Fe melt

temperature is 2000K



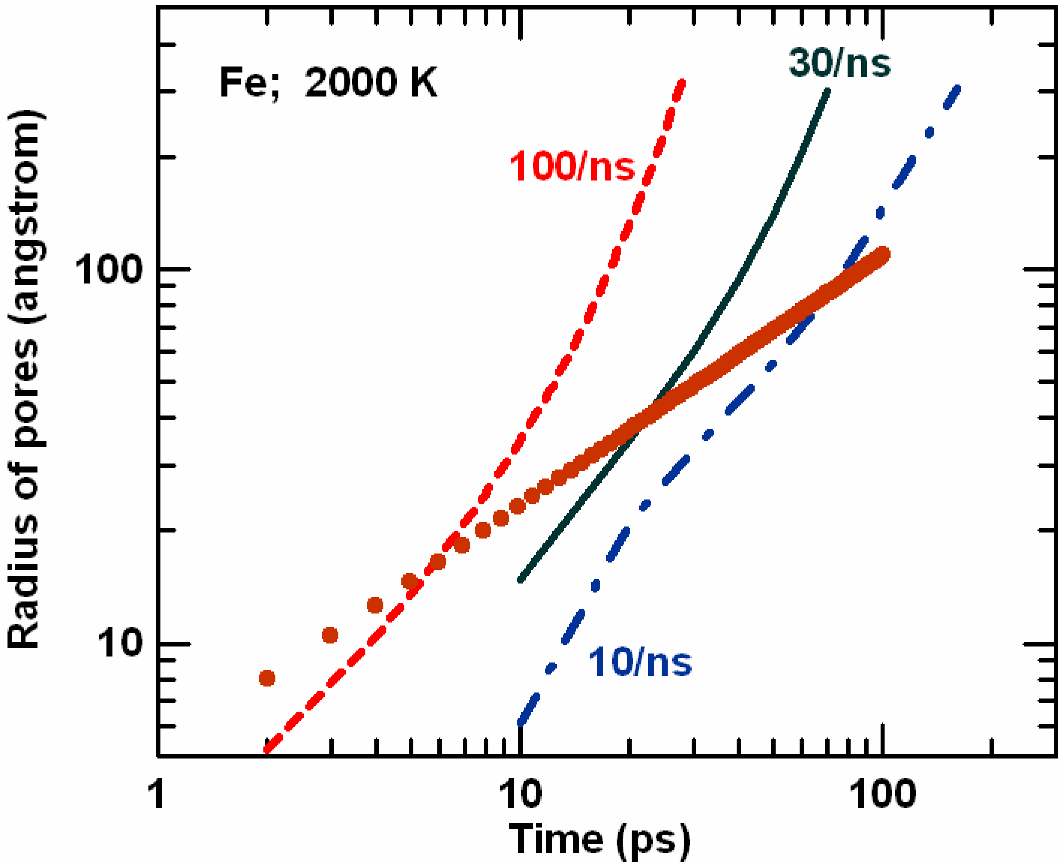
$$P = -\frac{2\sigma}{R_p}$$

$$\sigma = 1.017\ \mathrm{J/m^2}$$



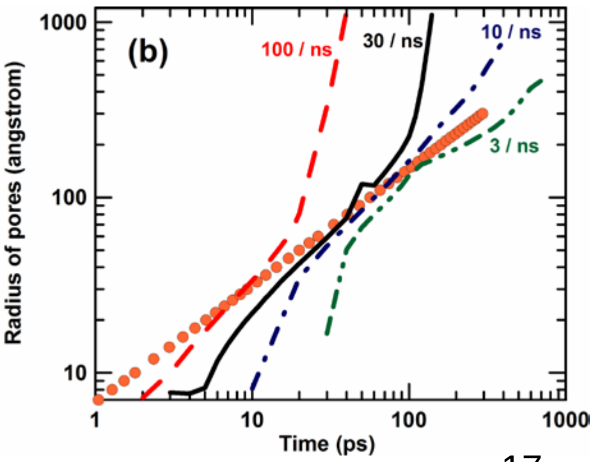
Evolution of pores in Fe melt at tension

temperature is 2000K



$$R_p = \frac{t^{2/3}\sigma^{1/3}}{\rho^{1/3}}$$

Al; 1100 K

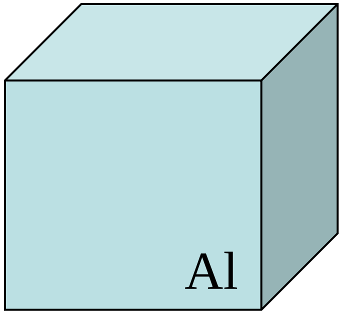


It is worse correspondence with analytical dependence for Fe melt than that for Al melt

Solidification of foamed Al melt

LAMMPS [Plimpton S. // J. Comp. Phys. (1995) http://lammps.sandia.gov]
OVITO [Stukowski A. // Modell. Simul. Mater. Sci. Eng. (2010) http://www.ovito.org]
"Construct surface mesh" algorithm [Stukowski A. // JOM (2014)]

4 000 000 atoms



Initial temperature is 2500 K to ensure melting

Cooling to 1100 K during 10 ps at zero pressure

Uniform tension with true strain rate of 30/ns during 50 ps:
final degree of deformation is 1.5 volume increases in 4.5 times

Two stages of cooling:

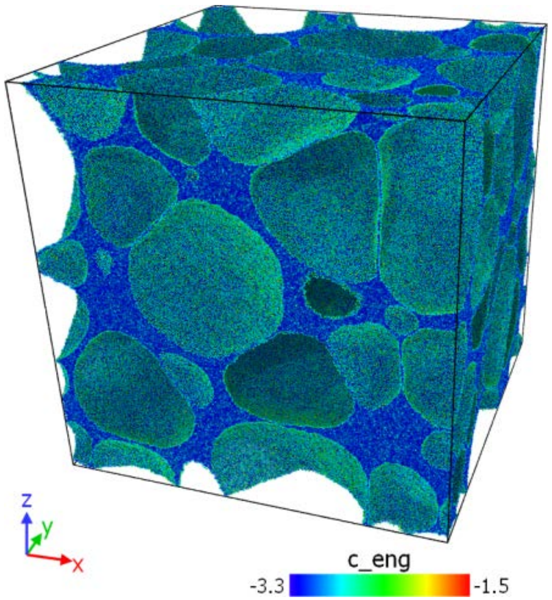
1. Cooling from 1100 to 500 K during 200 ps $\left(\frac{dT}{dt} = 3 \cdot 10^{12}\ \mathrm{K}^{-1} \right)$

2. Cooling from 500 to 300 K during 200 ps $\left(\frac{dT}{dt} = 10^{12}\ \mathrm{K}^{-1} \right)$

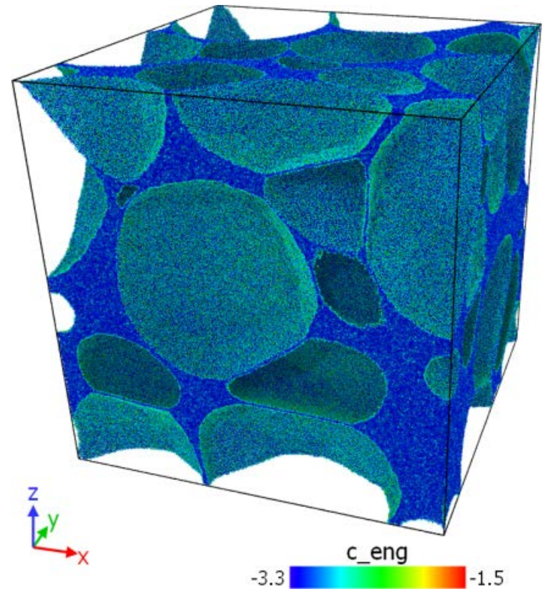
Interatomic potential for Al
[Zope R.R. and Mishin Y. // Phys. Rev. B. 68, 024102 (2003)]

Evolution of foamed structure in Al during the cooling of melt at constant volume

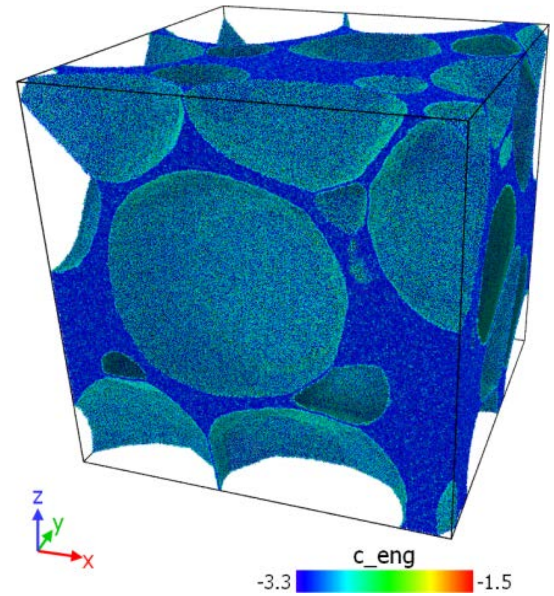
0 ps (1100 K)



50 ps (950 K)



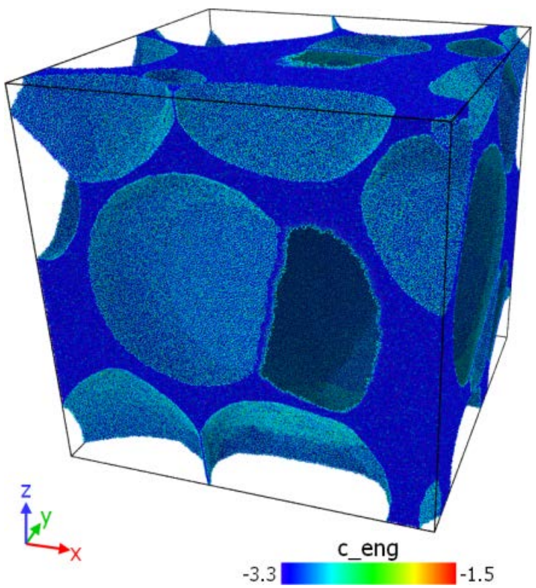
100 ps (800 K)



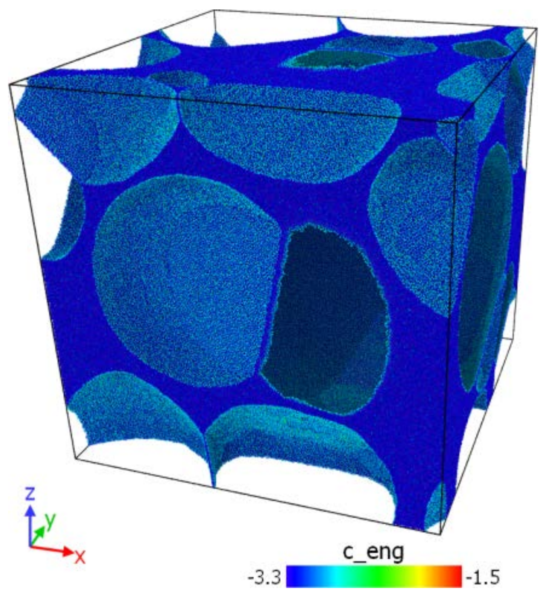
Growth of large cavities and collapse of small cavities instead of constant volume

Stabile form of cavities in Al at low temperatures

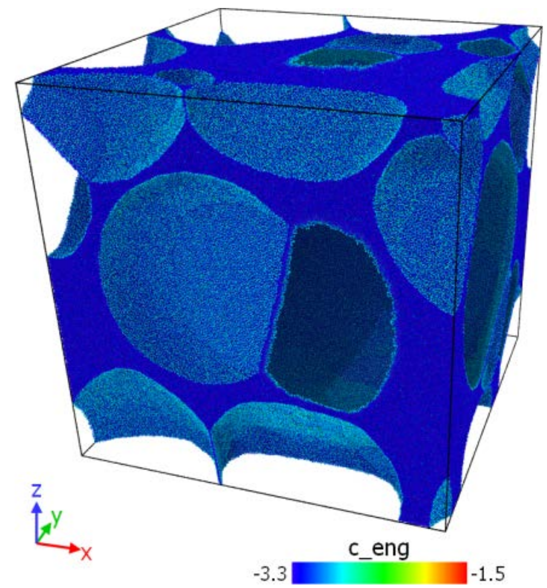
200 ps (500 K)



300 ps (400 K)



400 ps (300 K)



Stabile form argue that we obtain a solidified structure

Crystalline lattice is not detected

Week elastic properties are observed during subsequent uniaxial tension

Conclusions

1. Complete fracture of melt includes the following stages: (i) growth of large and collapse of small pores; (ii) destruction of walls between pores with formation of jets; (iii) fragmentation of jets on droplets.
2. The foamed melt retains till the void volume fraction exceeds 0.9 at least.
3. Pressure remains negative in the foamed melt at tension. The work required for complete fracture exceeds several times the work on reaching the cavitations point.
4. The foamed structure evolution is controlled by surface tension.
5. Analytical estimations for the time evolution of the mean radius, pressure in the system and the work on melt tension are proposed.
6. Simulation of the foamed melt cooling down to room temperature shows a solidified foamed metal structure formation, which persists over time.

Investigation of the pressure evolution in melt is supported by the Russian Science Foundation (Project No 14-11-00538); formation of the foamed structure is supported by the grant from the President of the Russian Federation (Project No. MK-9111.20167.8)