ANR MultiSil 13-BS09-0012

Multiscale methods for the analysis of plastic deformation of amorphous materials

Gergely Molnár

A. Tanguy, P. Ganster, G. Kermouche, E. Barthel

Content

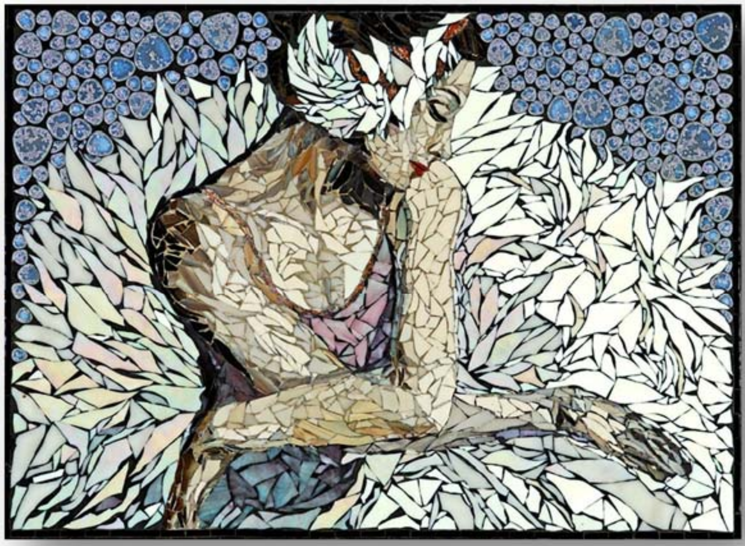
Initiation: Why Glass?

Multiscale mechanical approach:

1. **Atomic** scale deformation
2. **Microscopic** plasticity
3. Material **modeling**
4. **Experimental** comparison

Conclusion

Outlook



Laura Harris: Balerina
glass mosaic
2007

Why glass?

1282 → 1851 → 2012

Castello Nuovo

(Naples, Italy)

The Crystal Palace

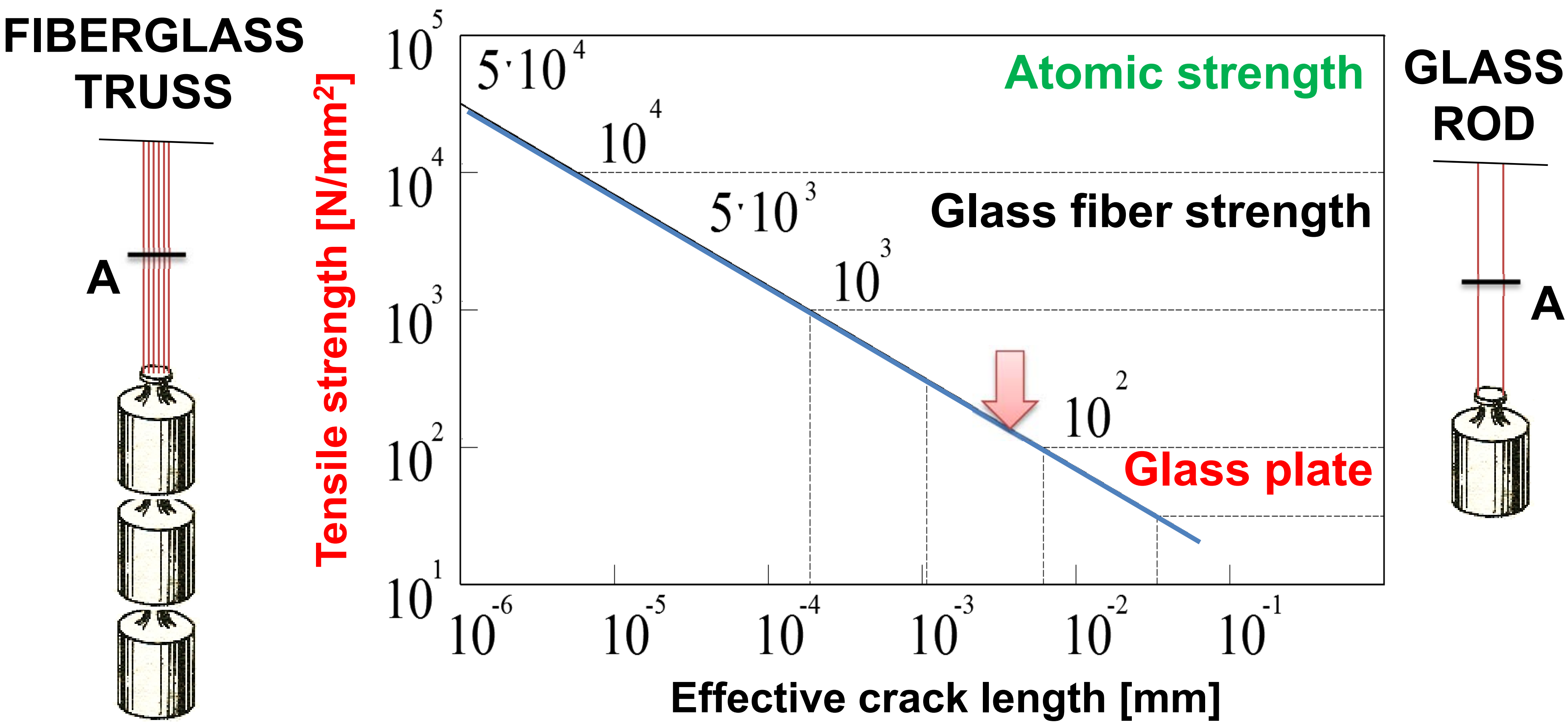
(London, UK)

Apple Cube

(New York City, USA)

Transparency with a high stiffness

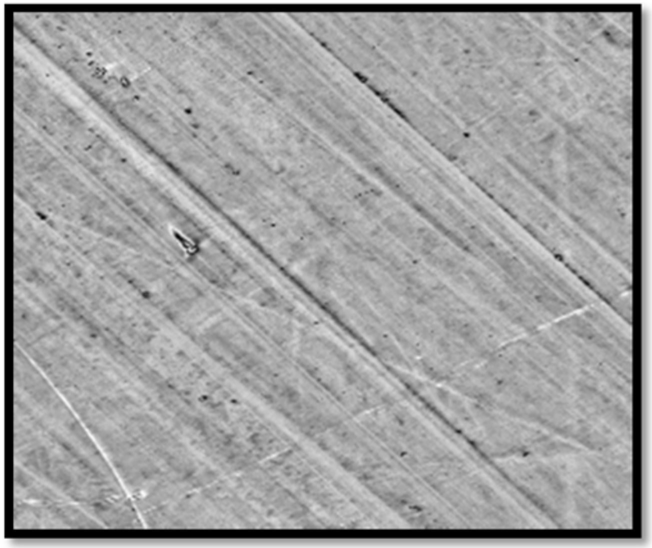
Macroscopic strength



J.-D. Wörner, Glasbau, 2001.

Initiation

Mesoscopic defects

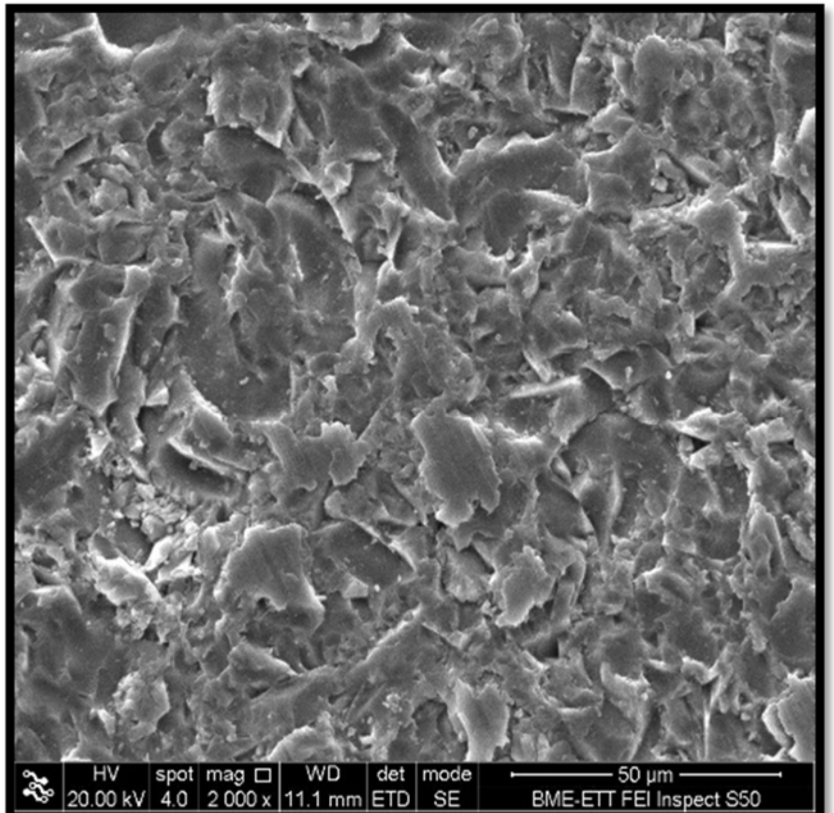


Glass surface

AFM image

Ground edge

SEM image

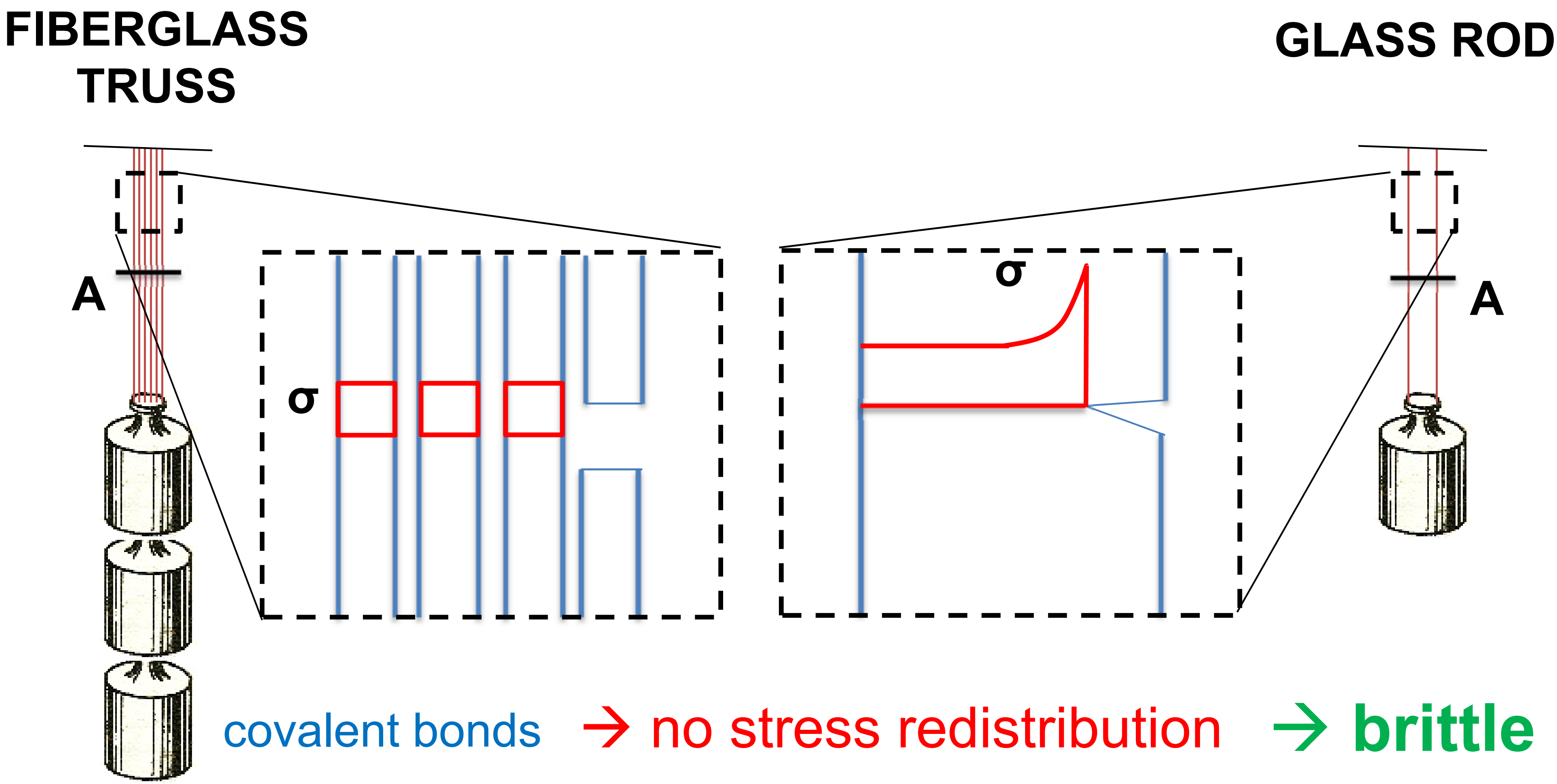


Bubbles

optical photo

G. Molnár et al., Mechanics of Materials, 2013

Macroscopic strength



covalent bonds → no stress redistribution → brittle

Brittle fracture

When and how does it break?

Intuitive testing methods

Bullet proof glass test

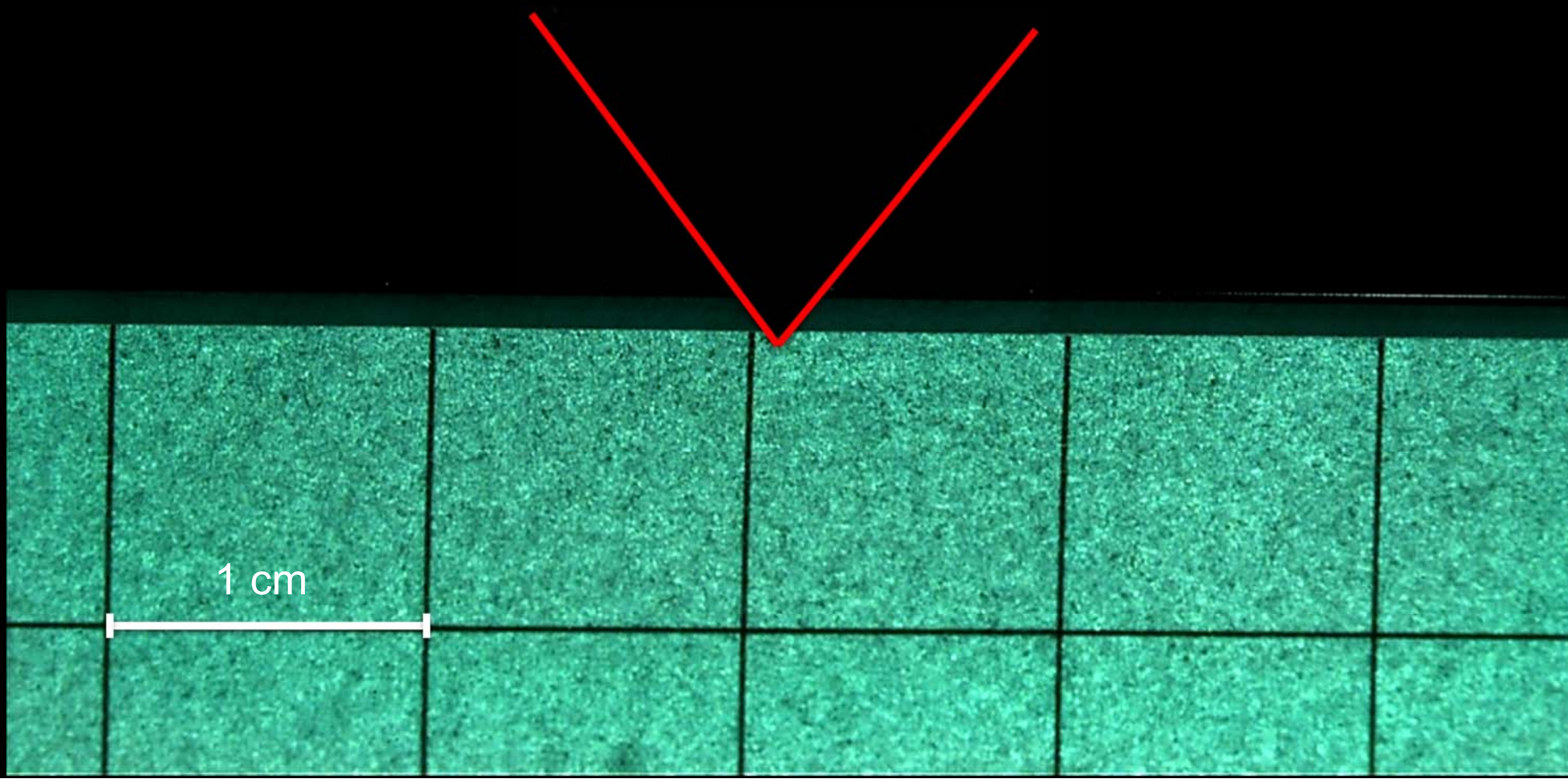
1952 (origin unknown)

Annealed glass plate

Resolution: 1280×1024 pixels

Speed: 100 fps

G. Molnár, Ph.D. Thesis, 2014

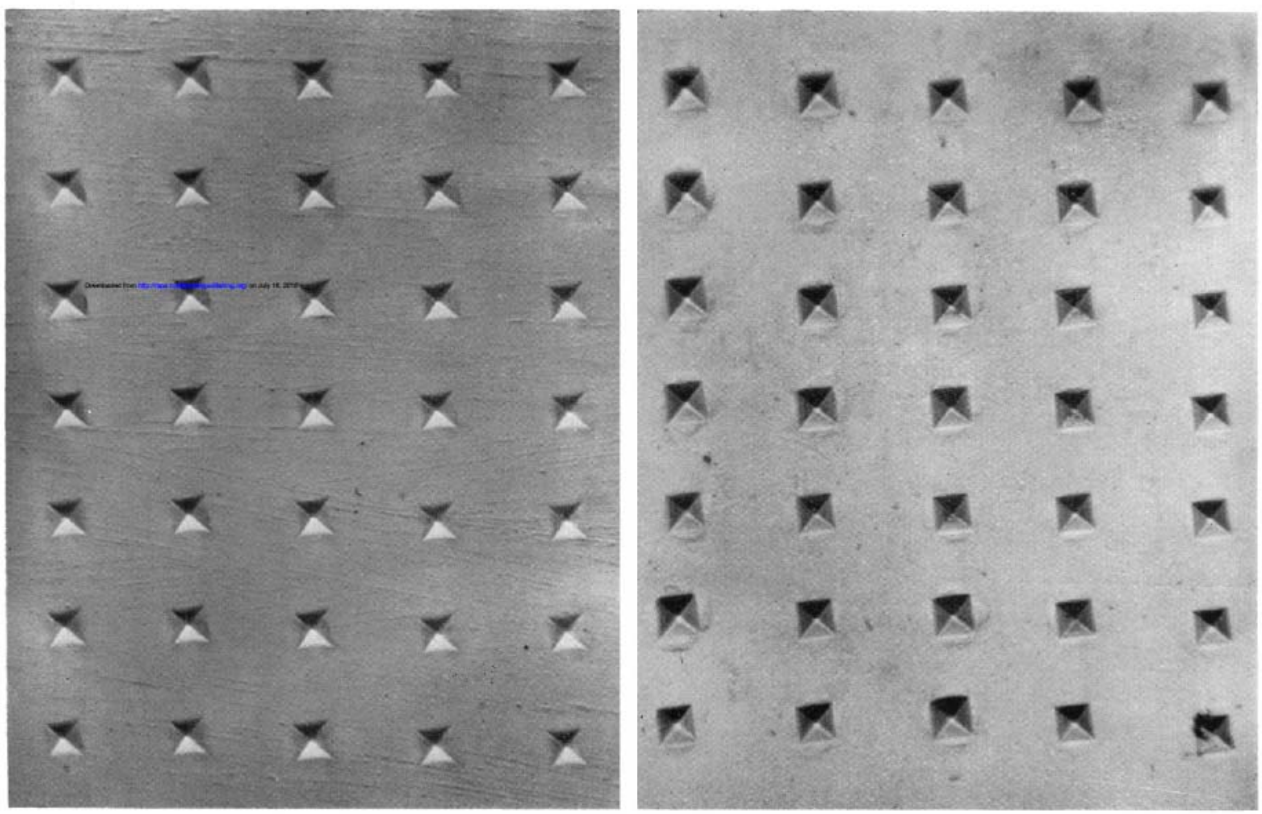


Initiation

Plasticity in silicate glasses

- 1949 : E.W. Taylor, Plastic deformation of optical glasses, ***Nature***.
- 1963 : D.M. Marsh, Plastic flow in glass, ***Proc. R. Soc. Lond. A***

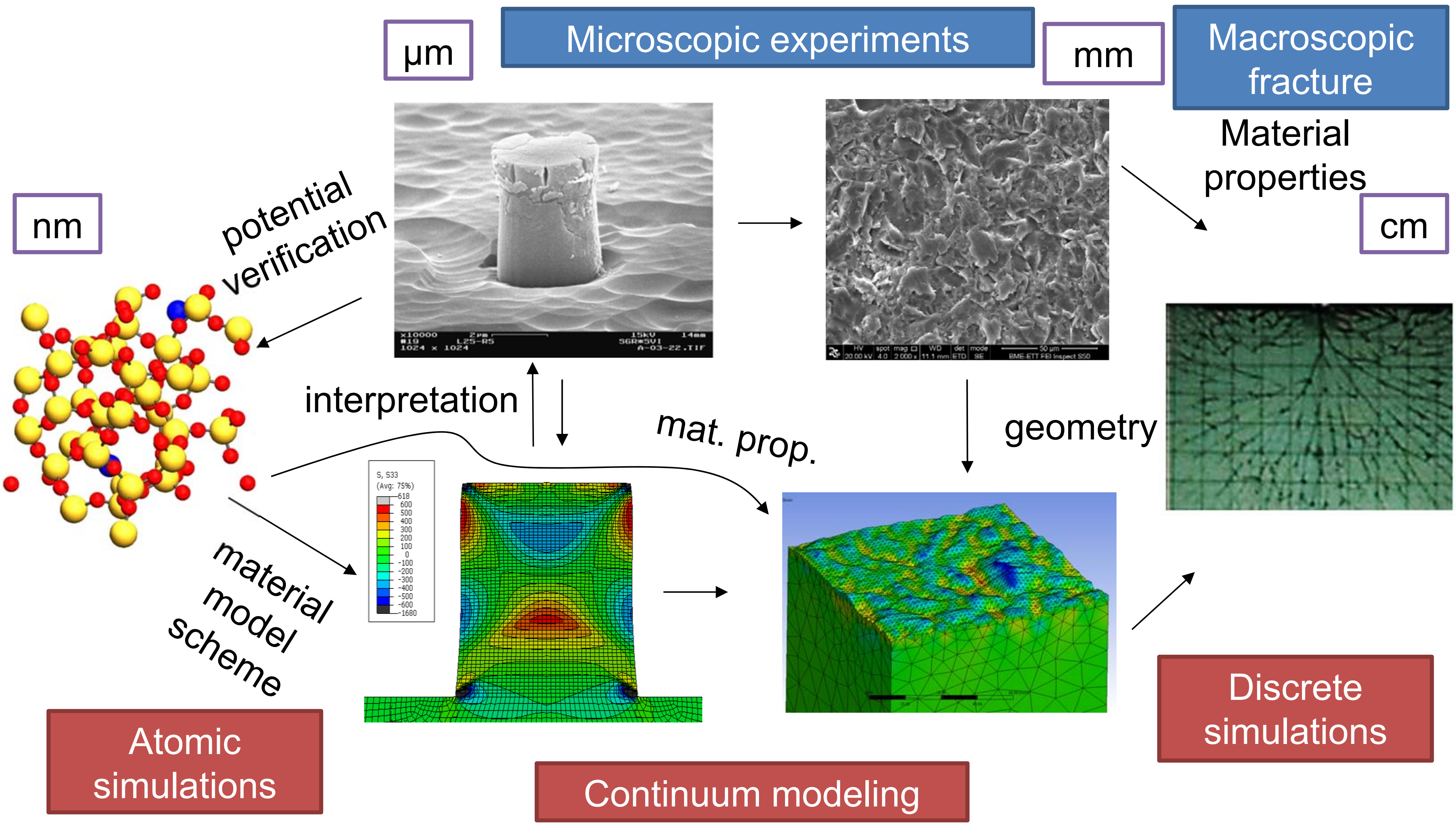
Window glass



Structural steel

FIGURE 2. Comparison of Vickers hardness impressions in glasses and in metals. (*Left*) in soda glass. (*Right*) in a bearing steel.

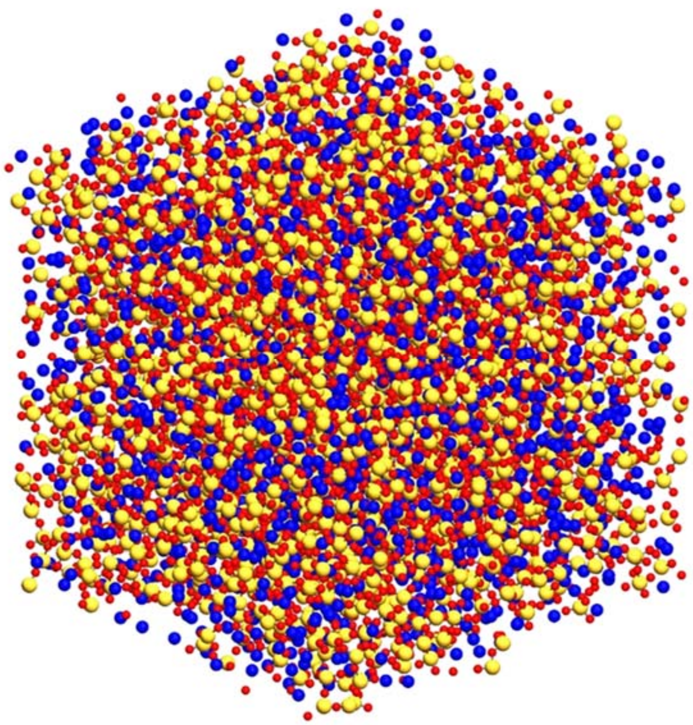
Multiscale approach



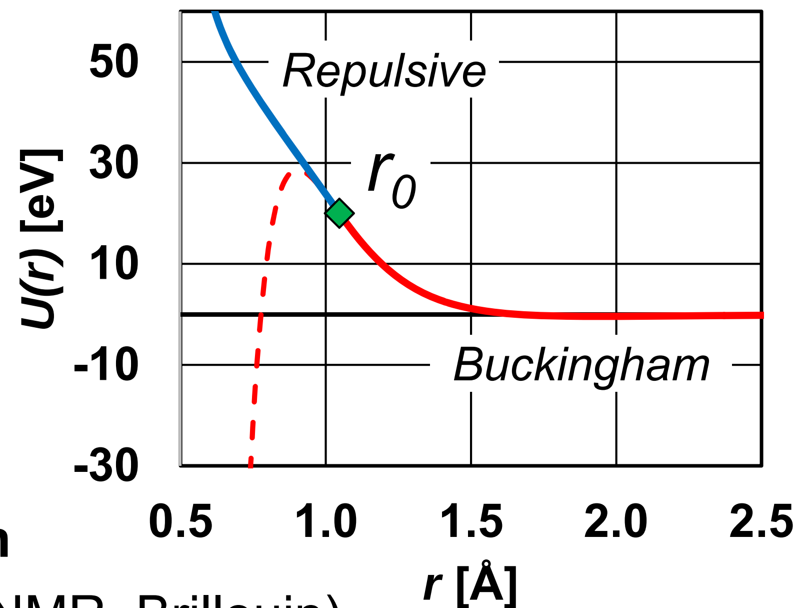
$$U_{BKS}\left(r_{ij}\right) = k\frac{q_i q_j}{r_{ij}} + e^{-r_{ij}/\rho} - \frac{C}{r^6}$$

Molecular dynamics

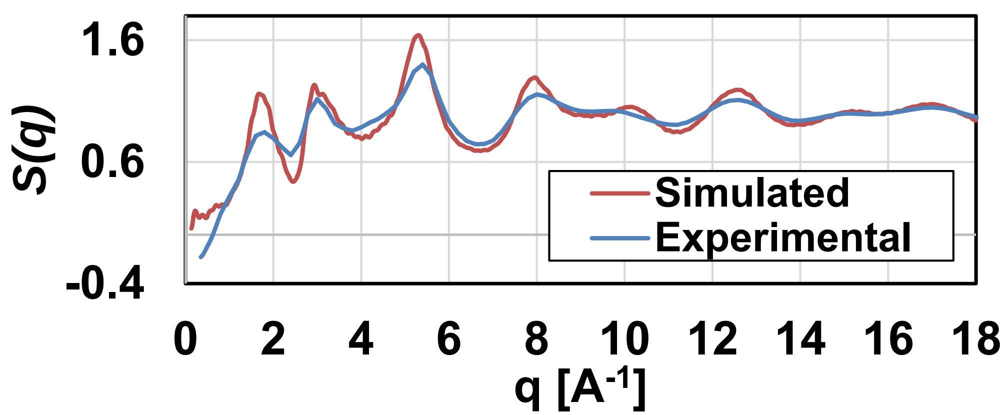
1. **BKS** Interaction potential
   (Cormack 2003)
2. Initial sample **generation**
   (random → heat → quench → SiO_2-xNa_2O)



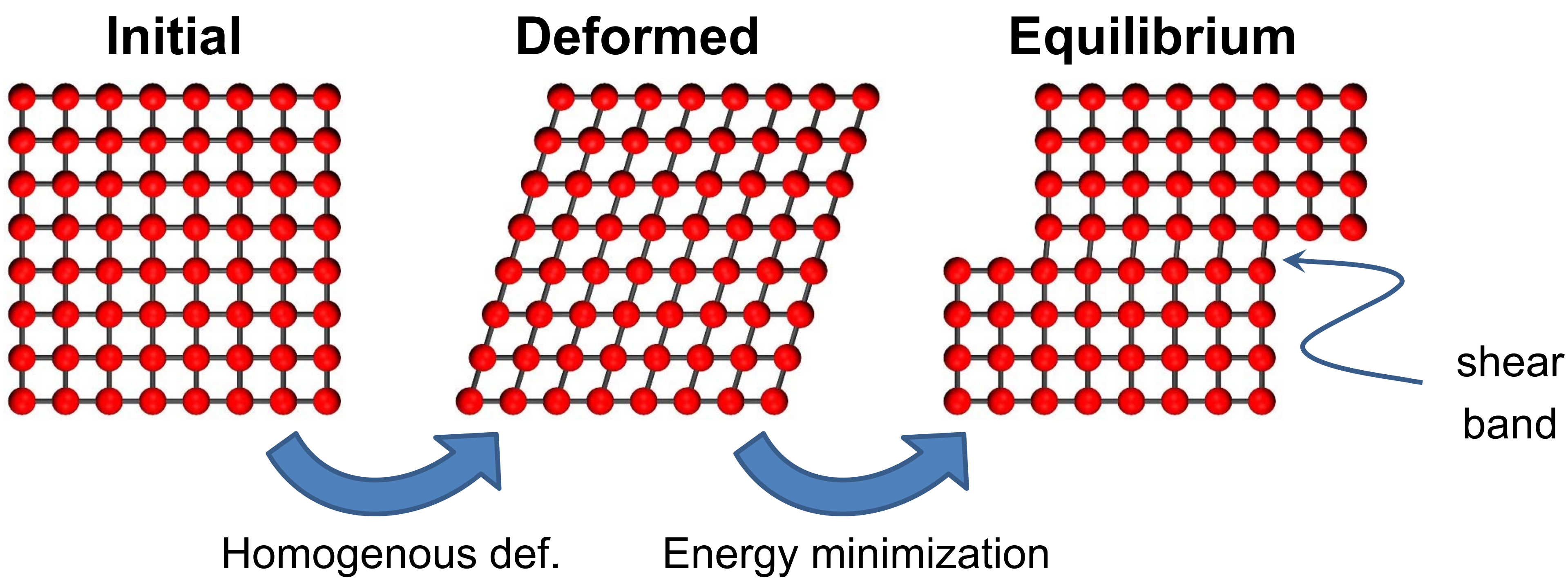
Potential function for Si-O



3. **Verification**
   (diffraction, NMR, Brillouin)



Atomic scale deformation (molecular statics)



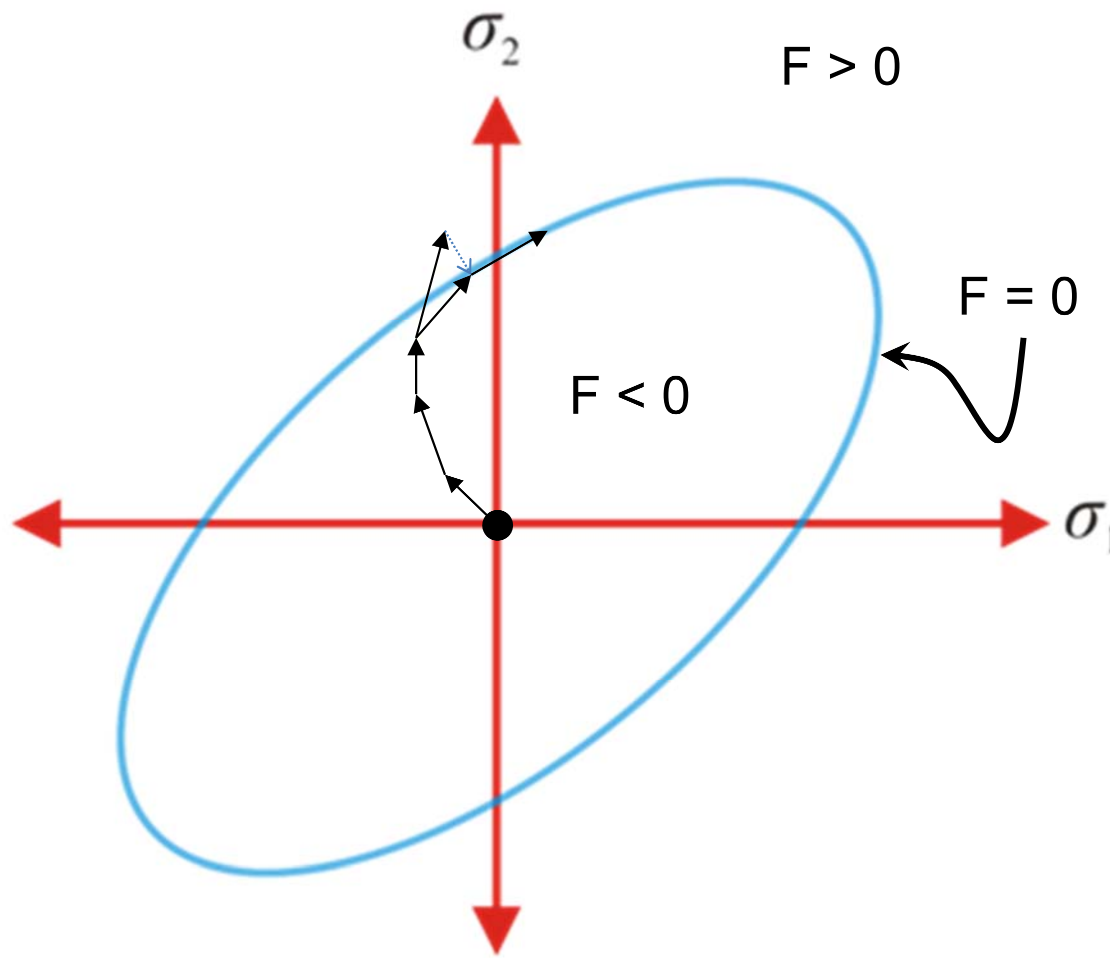
Stress

$$\boldsymbol{\sigma} = -\frac{1}{V}\sum_i \left[-m_i \boldsymbol{v}_i \otimes \boldsymbol{v}_i + \frac{1}{2}\sum_{i \neq j} \boldsymbol{r}_{ij} \otimes \boldsymbol{f}_{ij} \right]$$

Material model development

Basics (FEM)

1. Yield stress (*F*)
2. Elastic stress prediction (***K***)
3. Plastic return (dp^{pl})
4. Plastic strains ($d\varepsilon^{pl}$)
5. New yield stress



Computational plasticity (FEM)

1. Yield stress, stiffness (p_y)
2. Elastic stress prediction (K)
3. Plastic return (dp^{pl})
4. Plastic strains ($d\varepsilon^{pl}$)
5. New yield stress

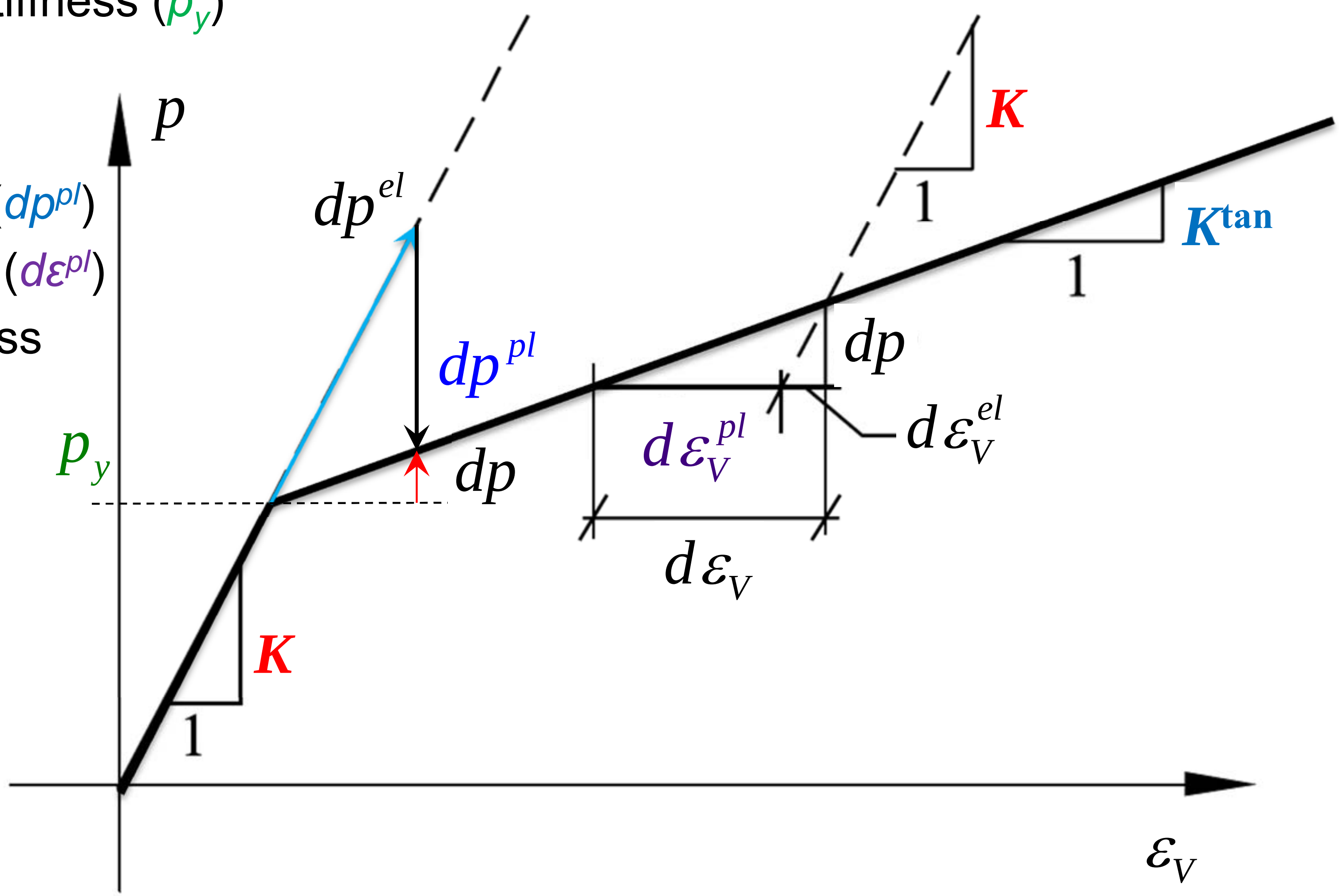
$$F = p - p^{y}\left(\varepsilon_V^{pl}\right) \leq 0$$

$$p^{y}\left(\varepsilon_V^{pl}\right) = p^{y,0} + H\varepsilon_V^{pl}$$

$$d\varepsilon_V = d\varepsilon_V^{el} + d\varepsilon_V^{pl}$$

$$dp = dp^{el} - dp^{pl}$$

$$dp^{pl} = Kd\varepsilon_V^{pl}$$

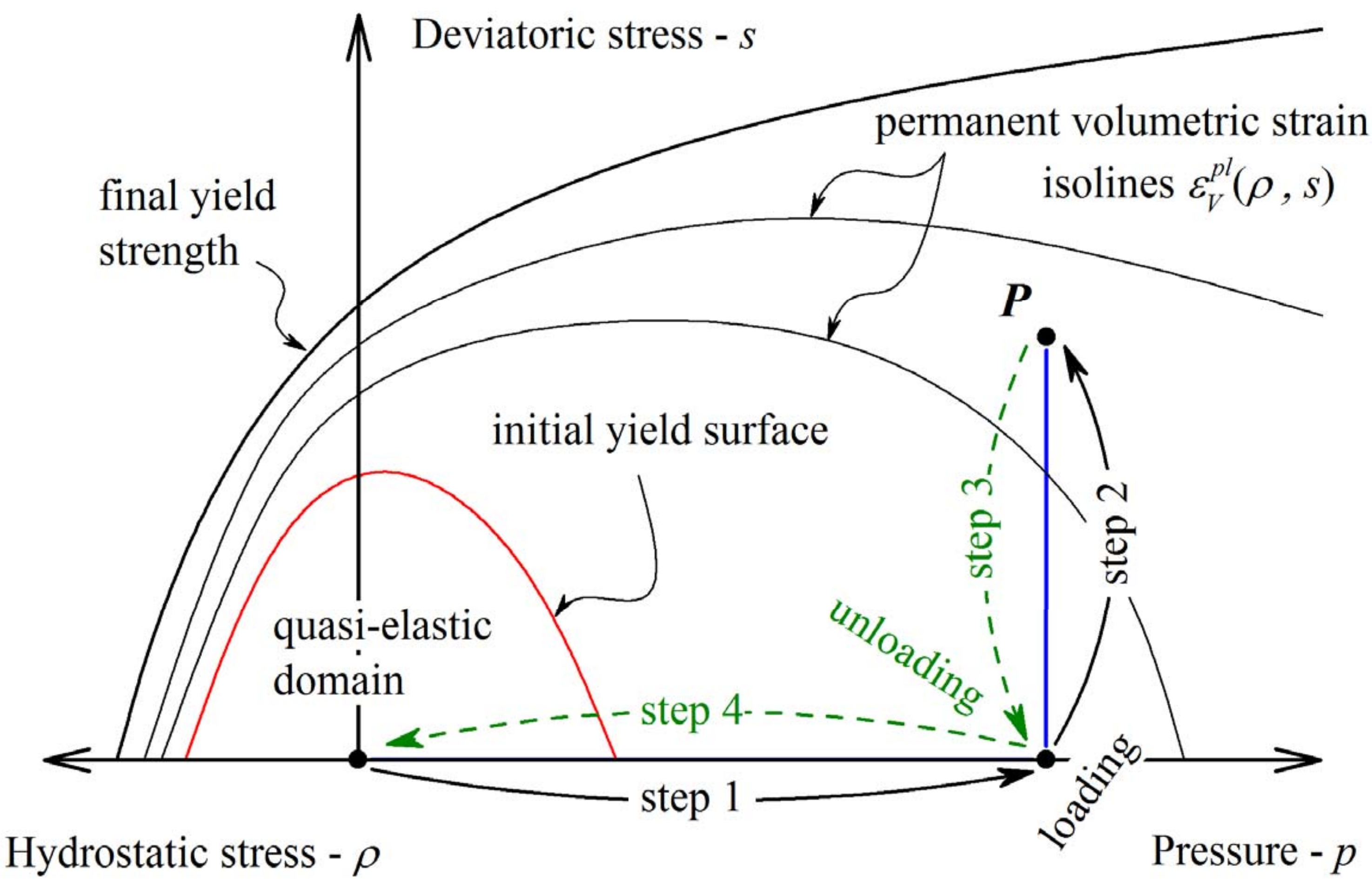


G. Molnár et al., Acta Materialia, 2016.

Material model development

MD/MS: Stress state → plastic strain

- quasi-static def.
- constant pressure shear



- implicit
- hardening plastic model

FEM: Plastic strain → Yield stress

Duality between MD/FEM

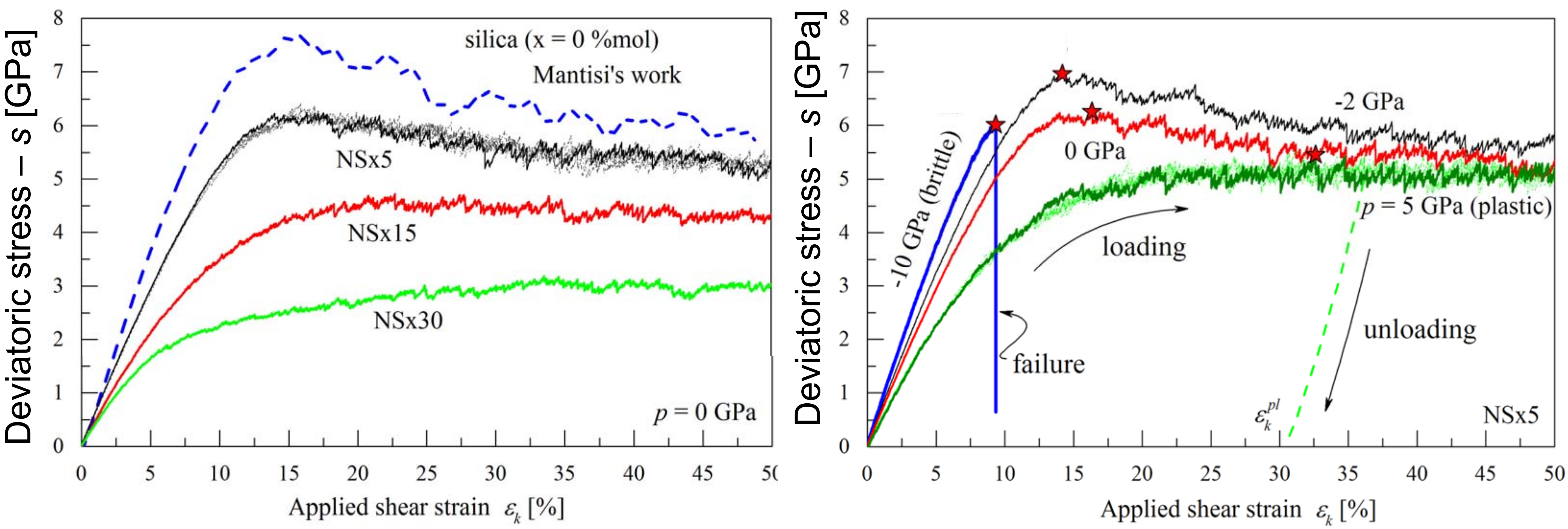
G. Molnár et al., PRE, 2017.

Atomistic response

Shear stress results

Composition

Pressure state



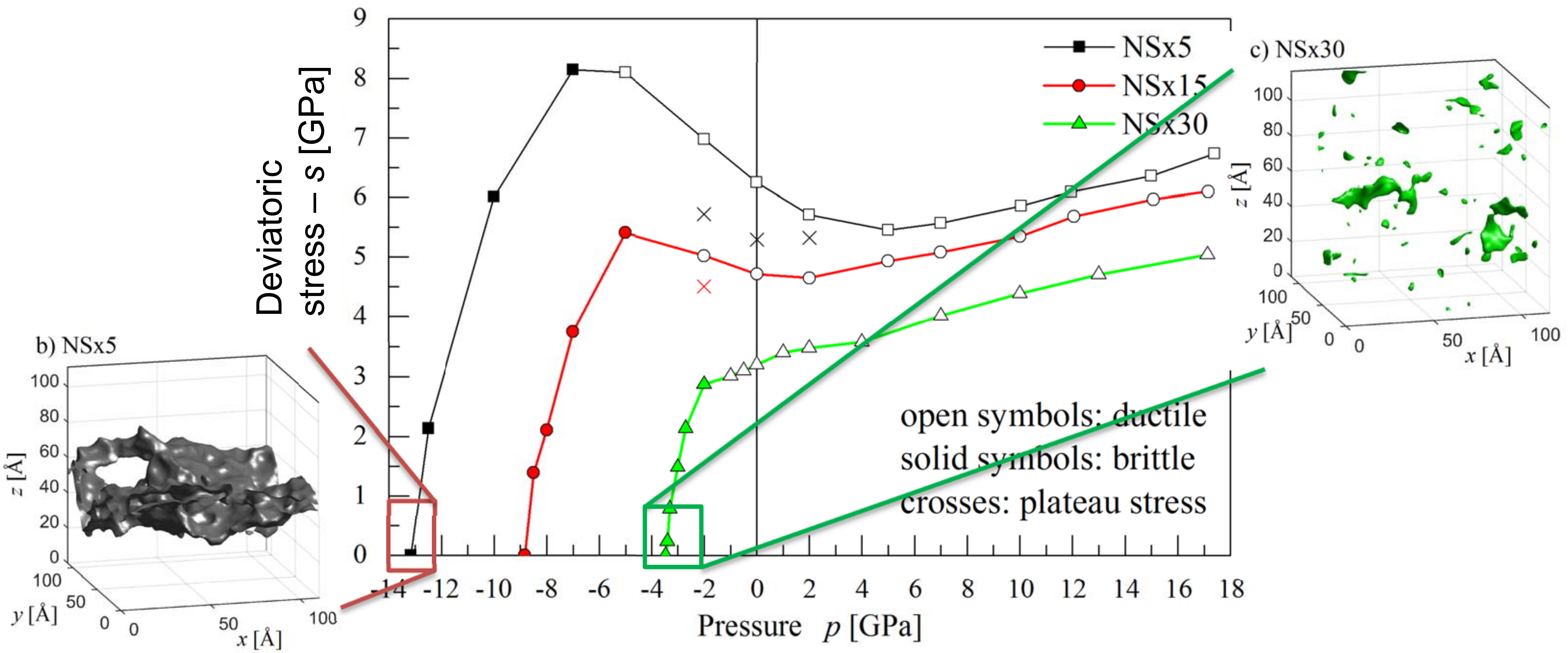
G. Molnár et al., PRE, 2017.

Atomistic response

Shear stress results

Composition

Pressure state

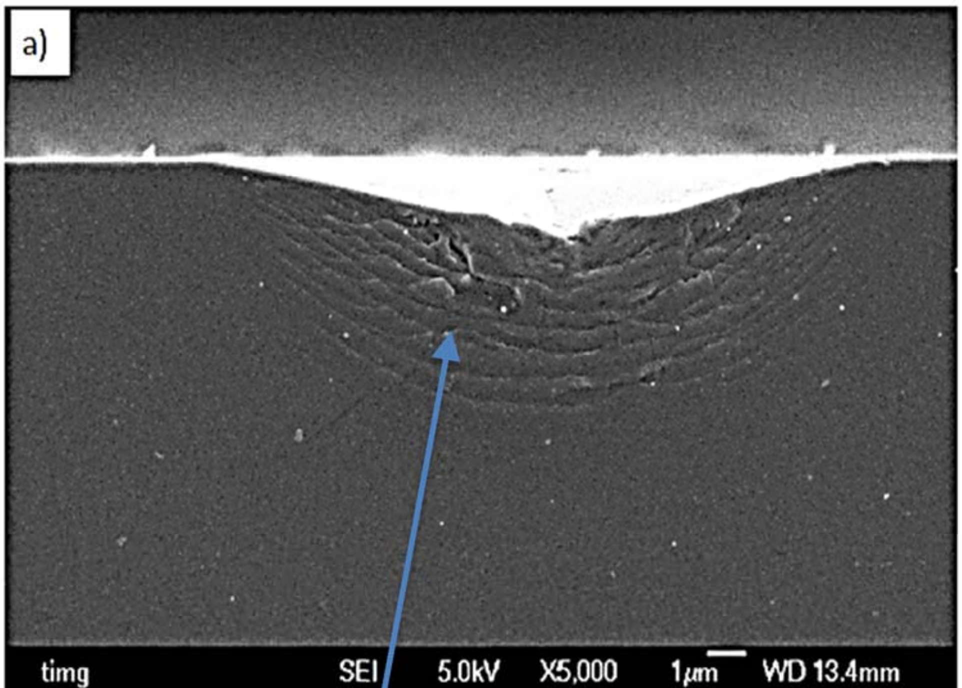


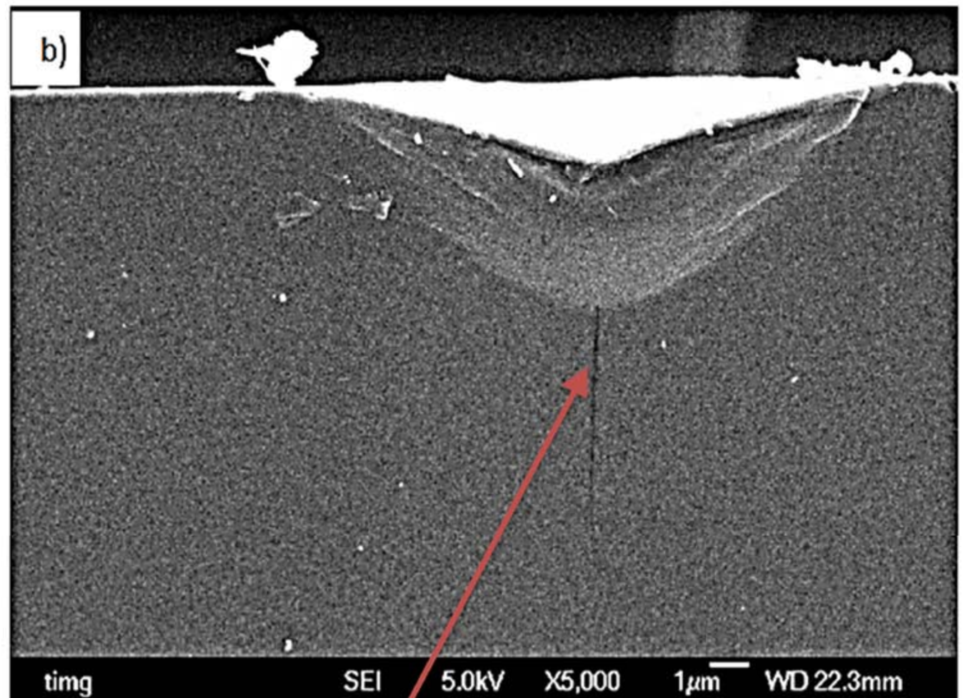
Atomistic response

Brittle vs plastic?

Sodium silicate
ductile

Silica
fragile





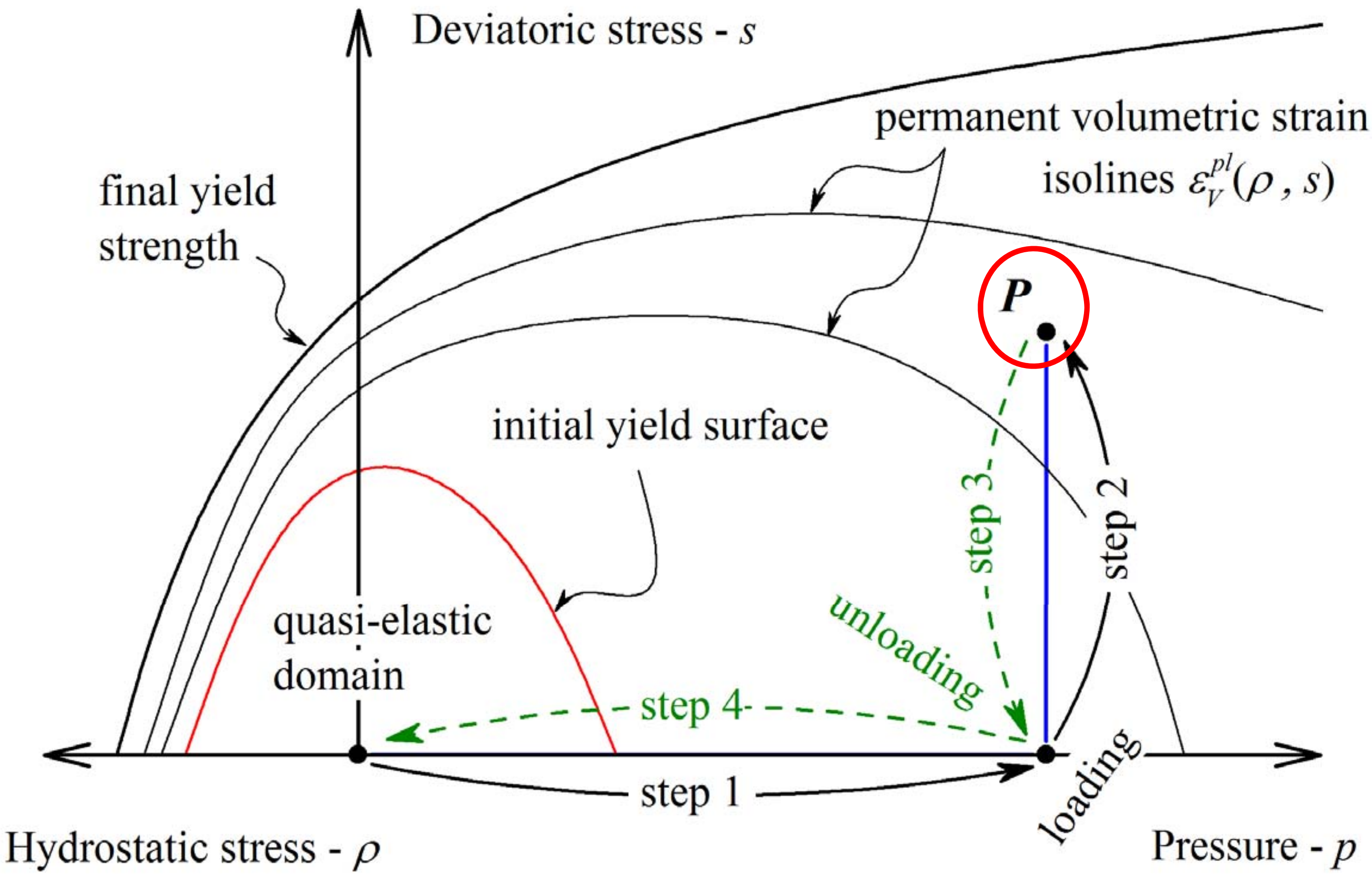
ductile regime

fragile crack

G. Molnár et al., Acta Materialia, 2016.

Material model development

MD/MS: Stress state → plastic strain



- quasi-static def.
- constant pressure shear

- implicit
- hardening plastic model

FEM: Plastic strain → Yield stress

Duality between MD/FEM

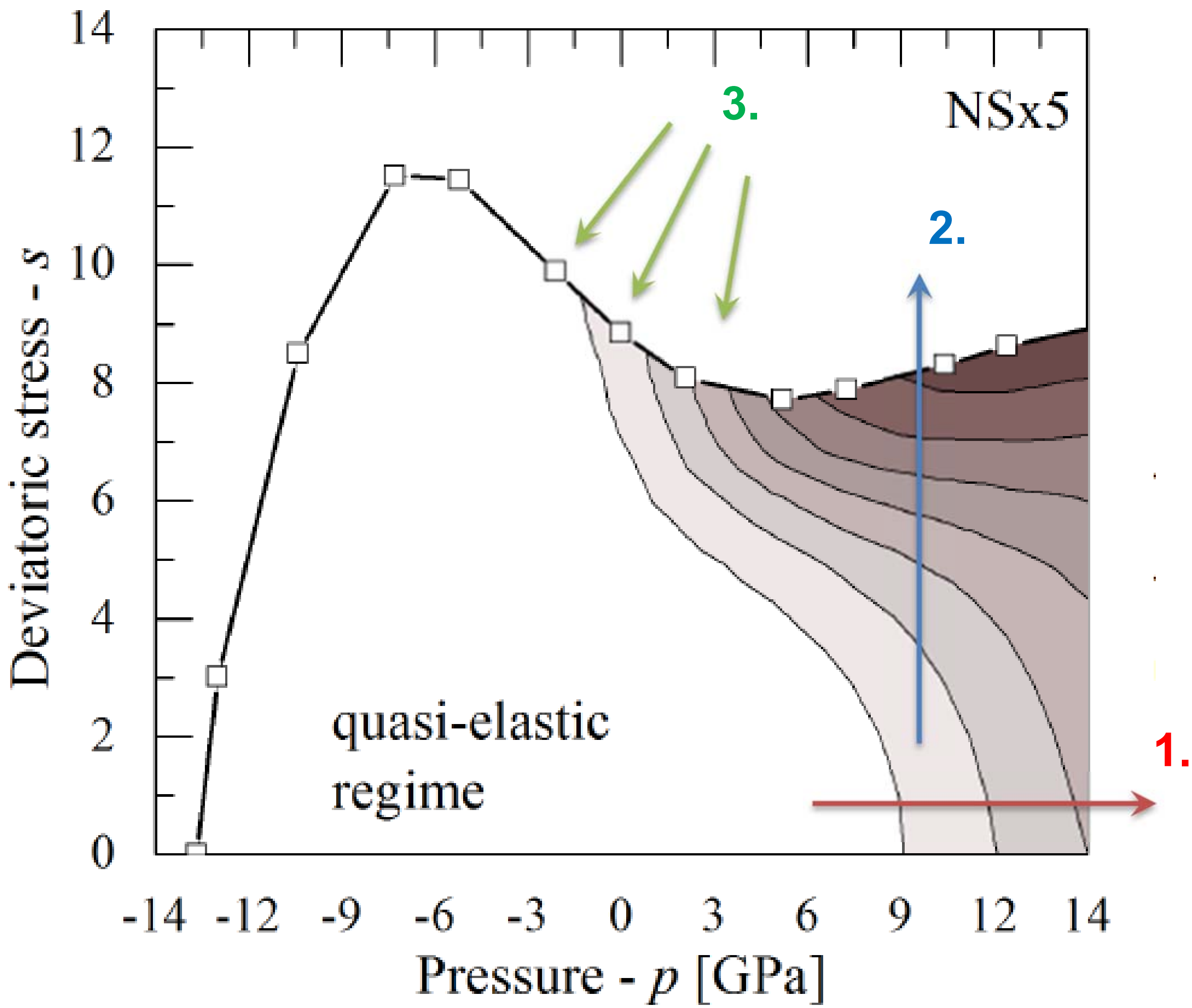
G. Molnár et al., Acta Materialia, 2016.

Atomistic response

Densification (permanent volume change)

$$\varepsilon_V^{pl} = \varepsilon_z^{pl} + \varepsilon_y^{pl} + \varepsilon_z^{pl}$$

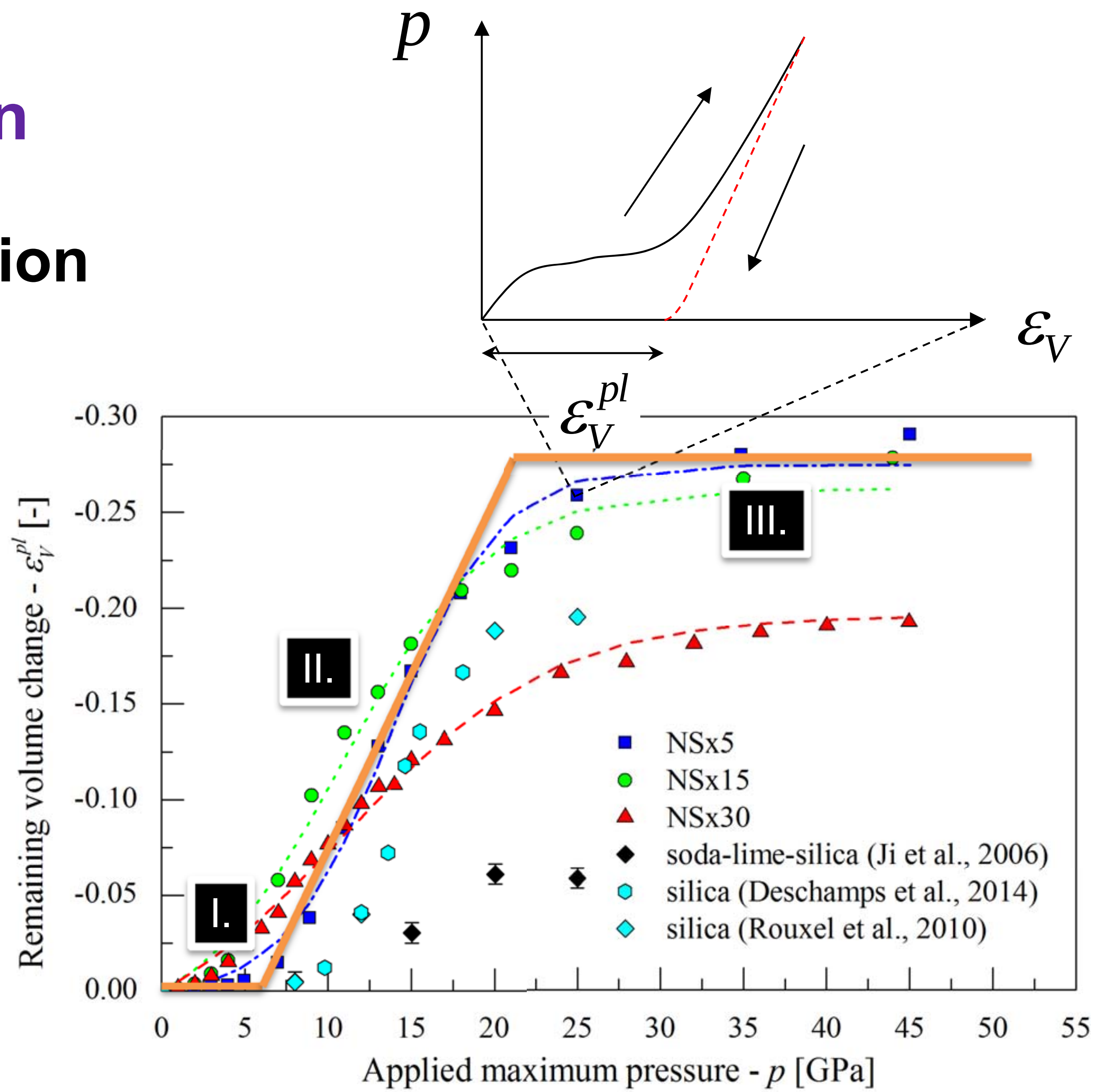
Hencky-logarithmic strain



Unprocessed results

Densification

Hydrostatic compression



Hydrostatic plastic strain increases in a sigmoidal way

G. Molnár et al., Acta Materialia, 2016.

Densification

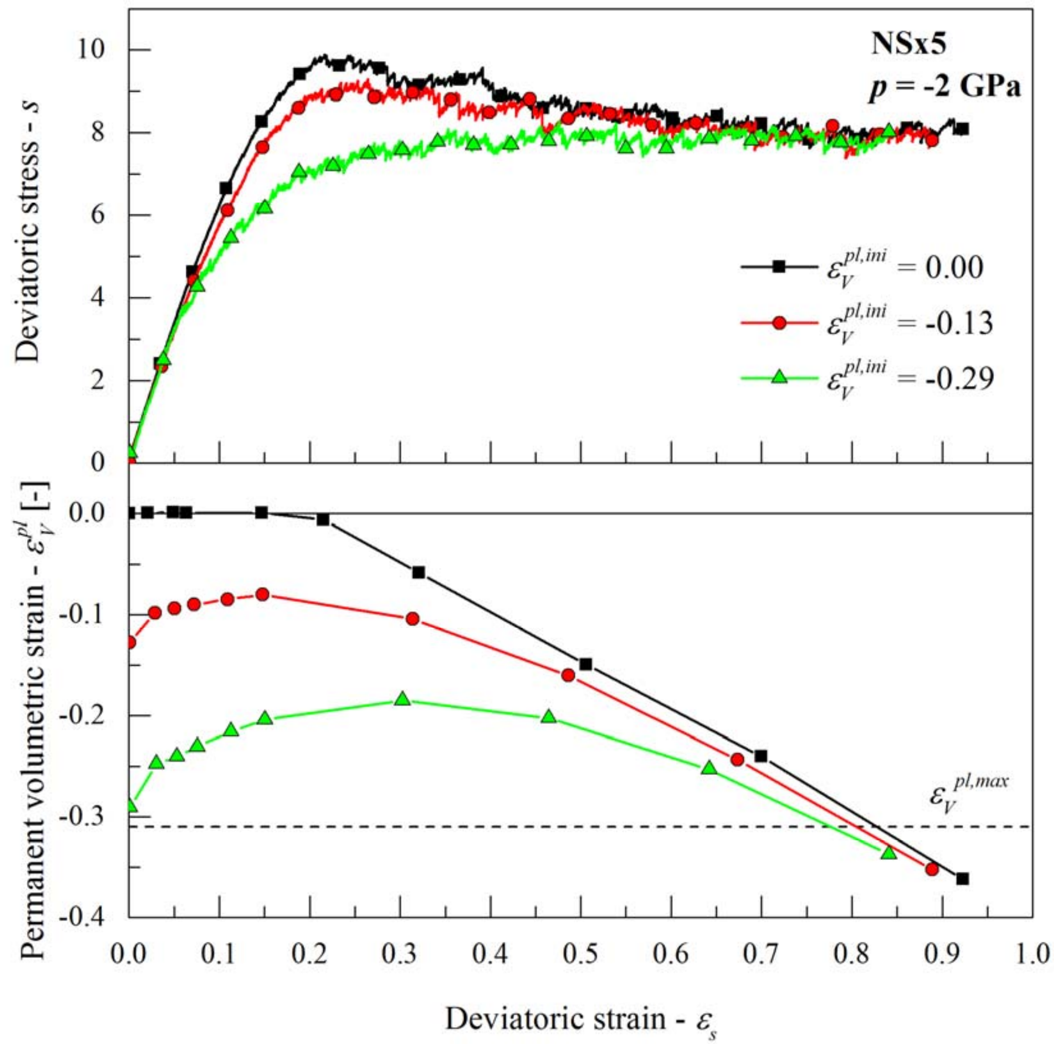
Shear at constant pressure

Deviatoric component

$$\varepsilon_V^{pl} = \varepsilon_V^{pl,0} + Bs_\varepsilon^{pl}$$

Damage variable

Real hydrostatic strain

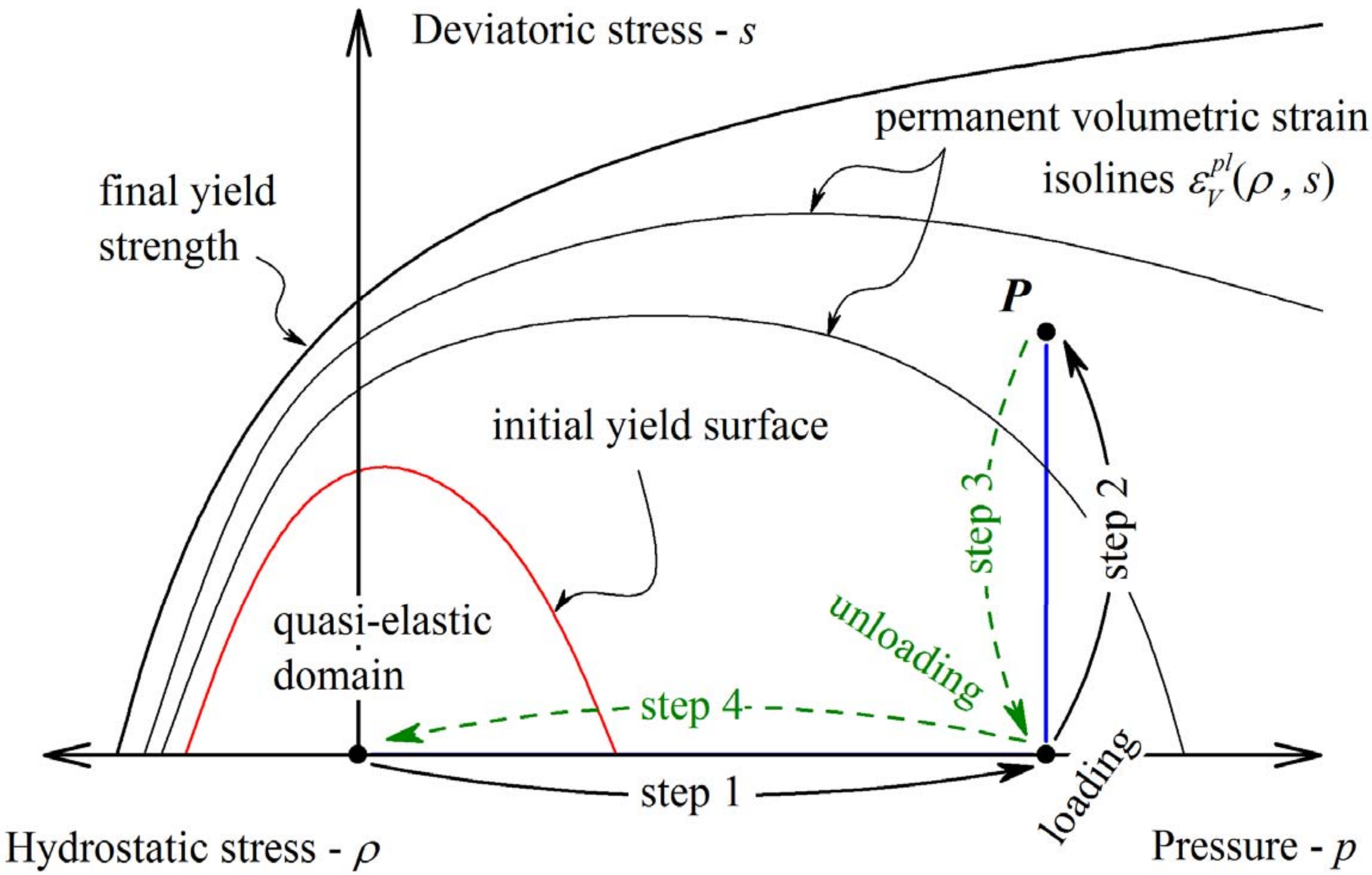


Densification upon shear at constant pressure

G. Molnár et al., Acta Materialia, 2016.

Atomistic response

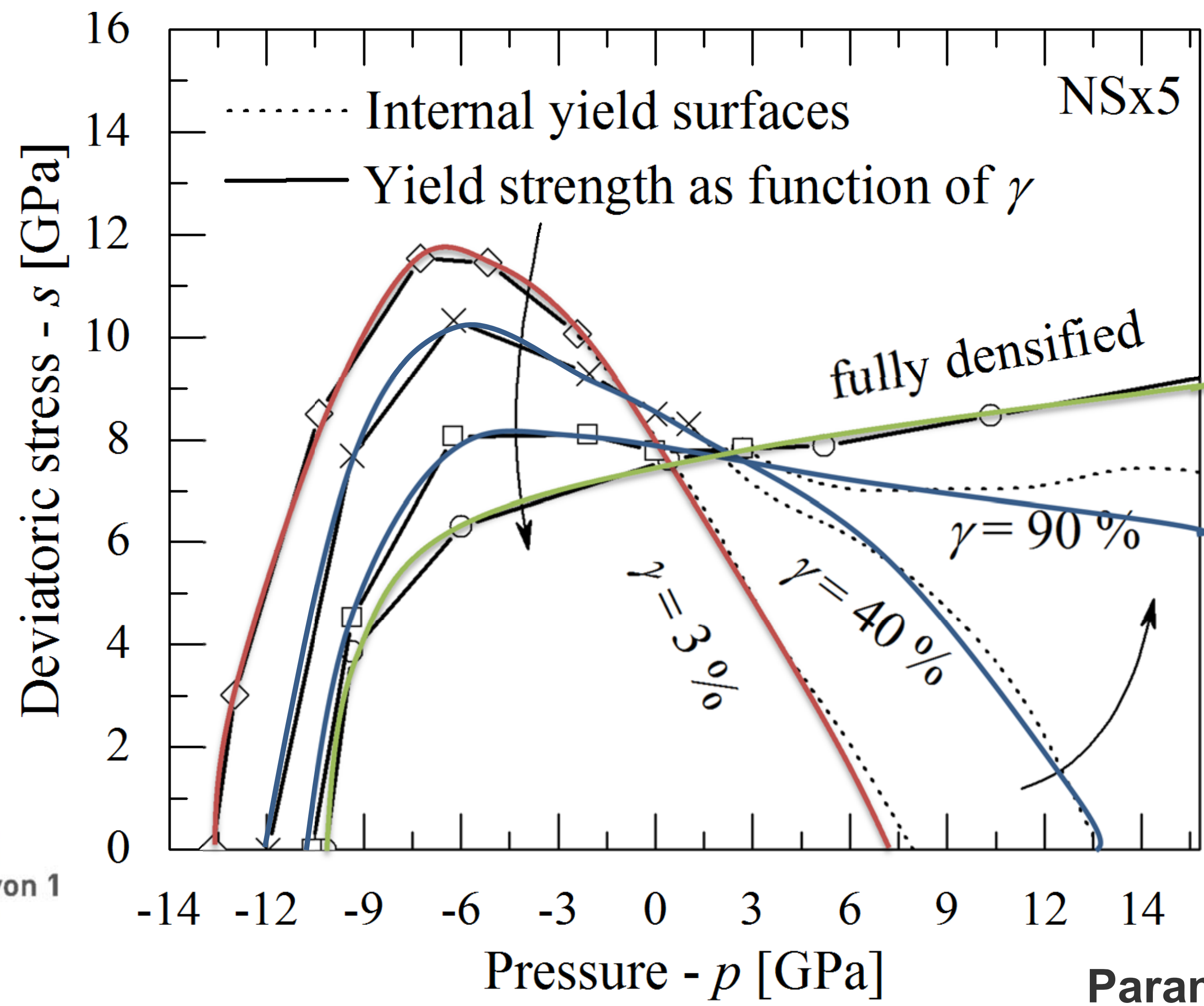
MD: Stress state → plastic strain



FEM: Plastic strain → Yield stress

Pre-densification

Atomistic response

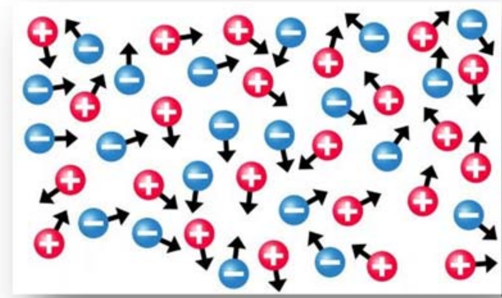


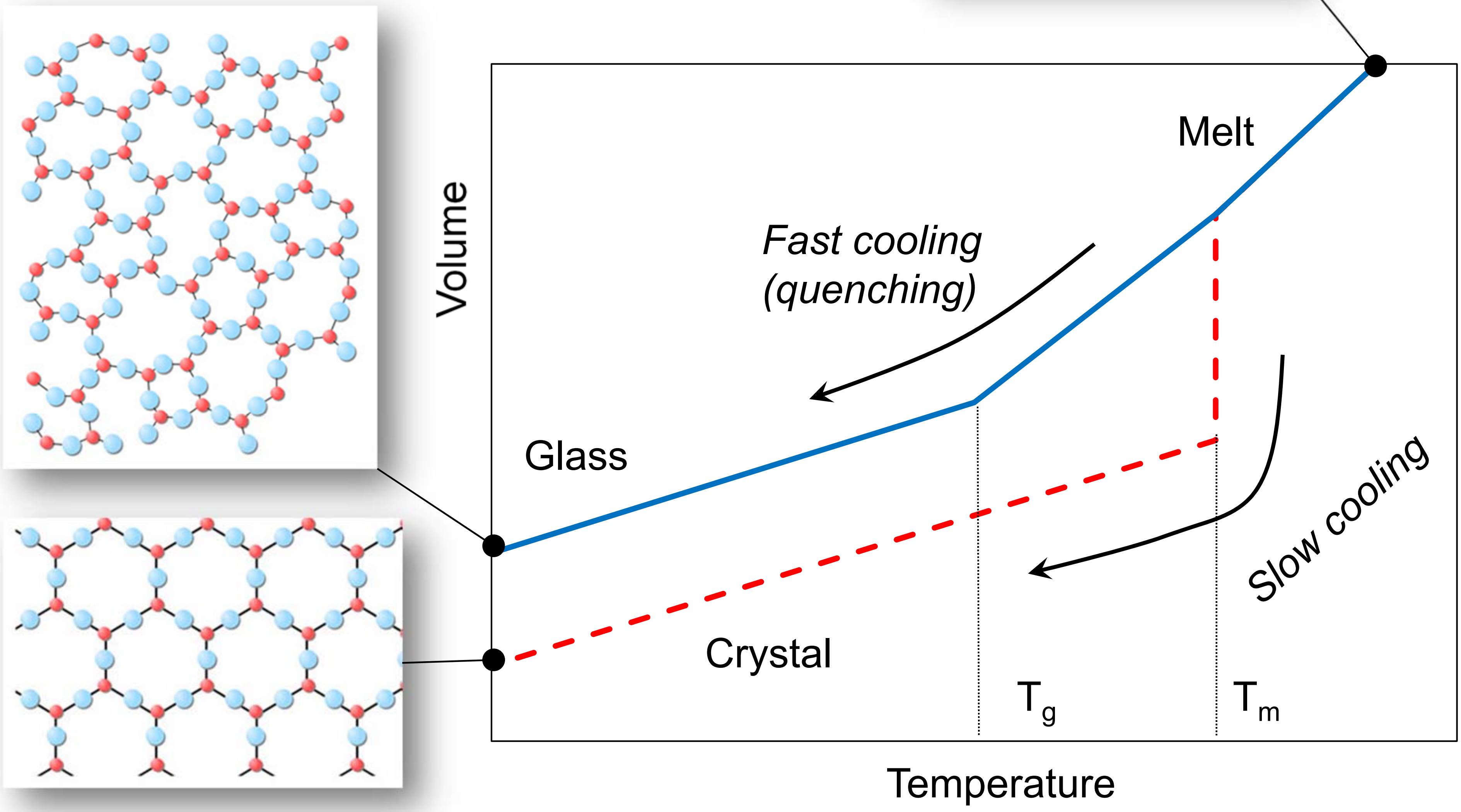
$$\gamma = \frac{\varepsilon_V^{pl}}{\varepsilon_V^{pl,\max}}$$

Parameterized by density

What is glass?

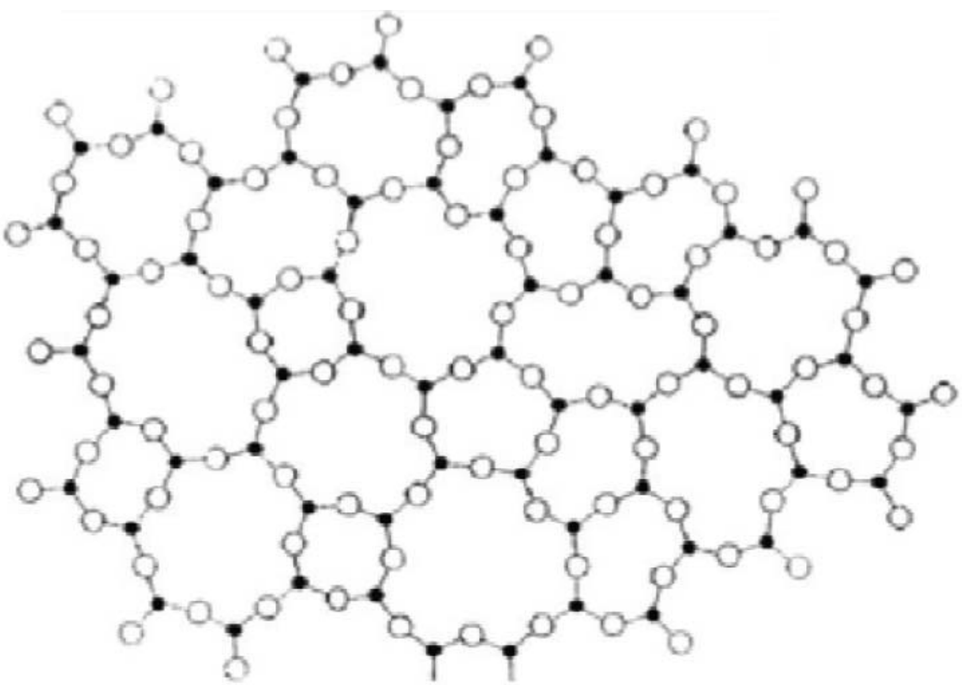
Amorphous silica





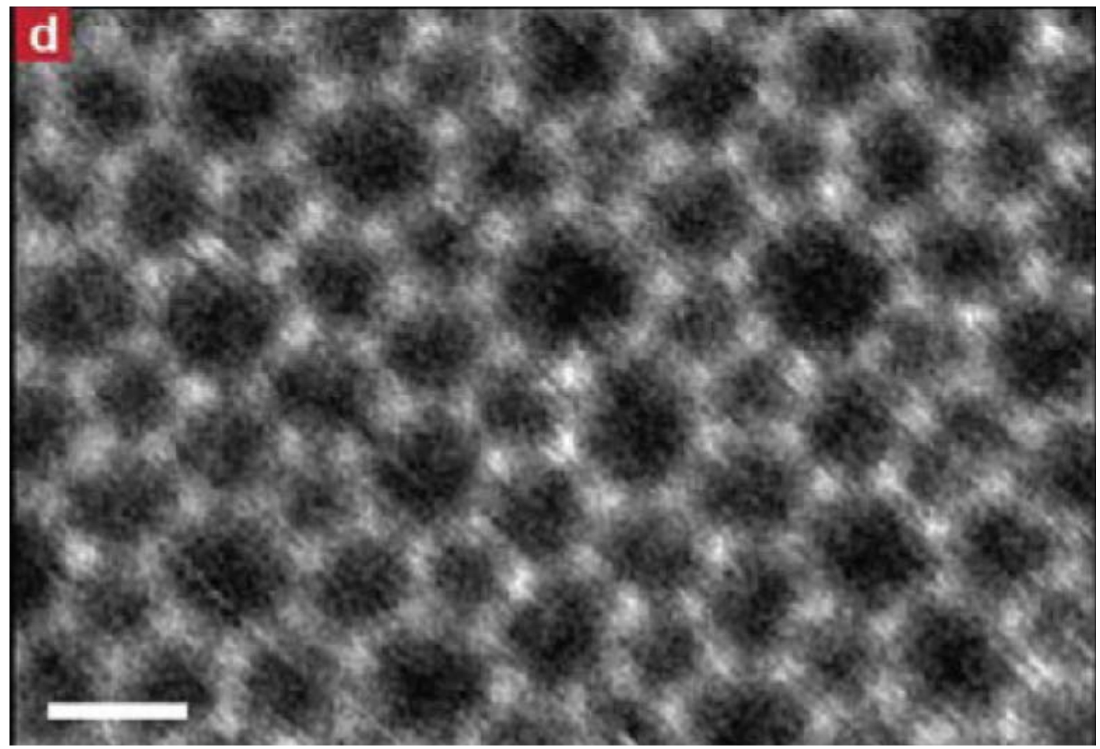
Amorphous silica

Zachariasen's original concept (1932)



Open atomic structure

Atomic-resolution electron spectroscopy

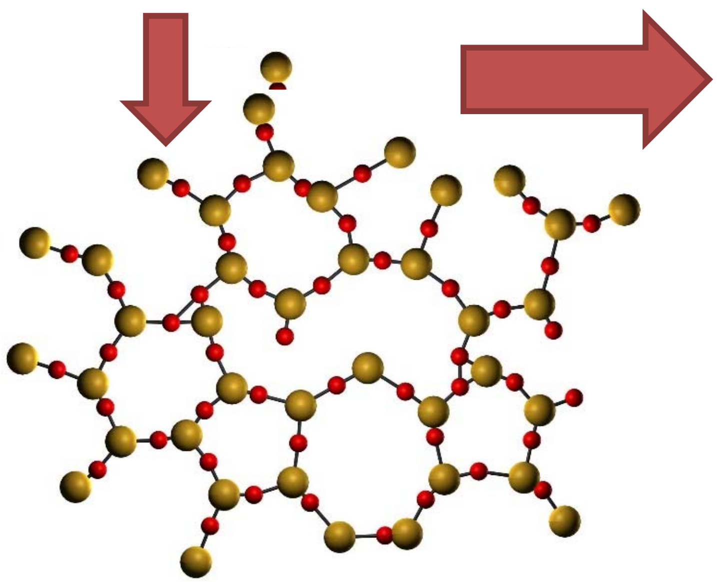


P. Y. Huang et al., NL, 2012.

What is glass?

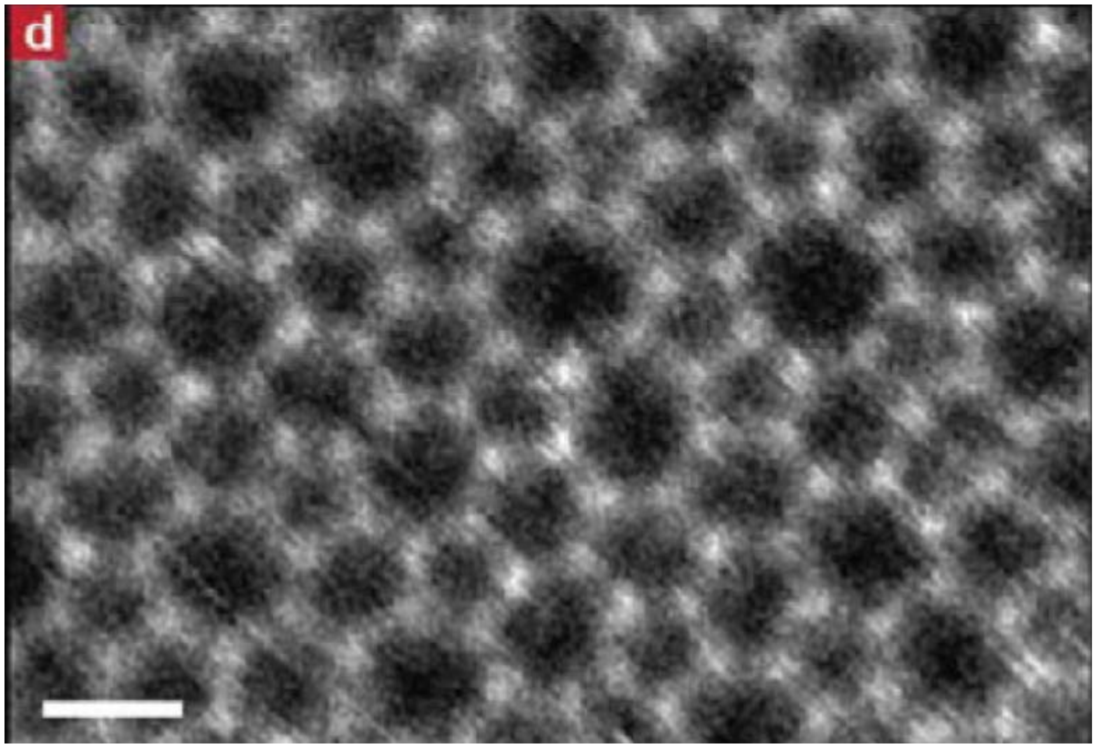
Amorphous silica

Shear transformation zone
Plastic event



Open atomic structure

Atomic-resolution electron spectroscopy

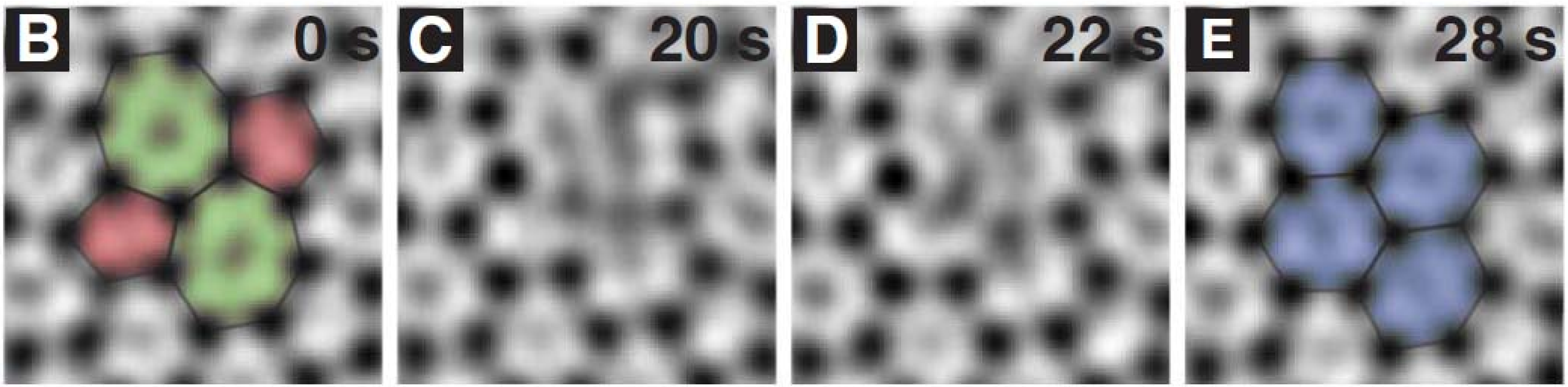


P. Y. Huang et al., NL, 2012.

Amorphous silica

Shear transformation zone
Plastic event

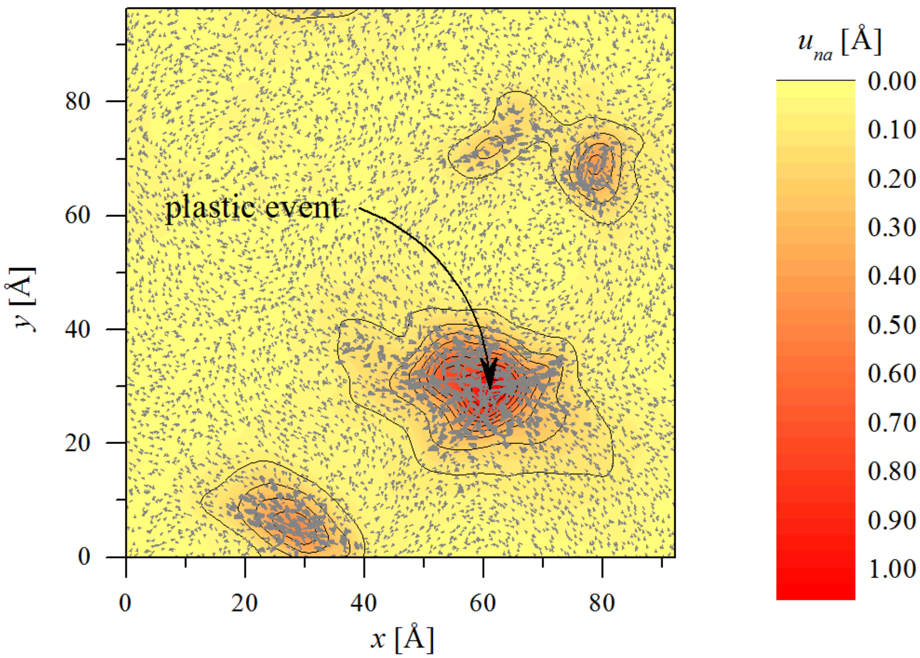
Atomic-resolution electron spectroscopy

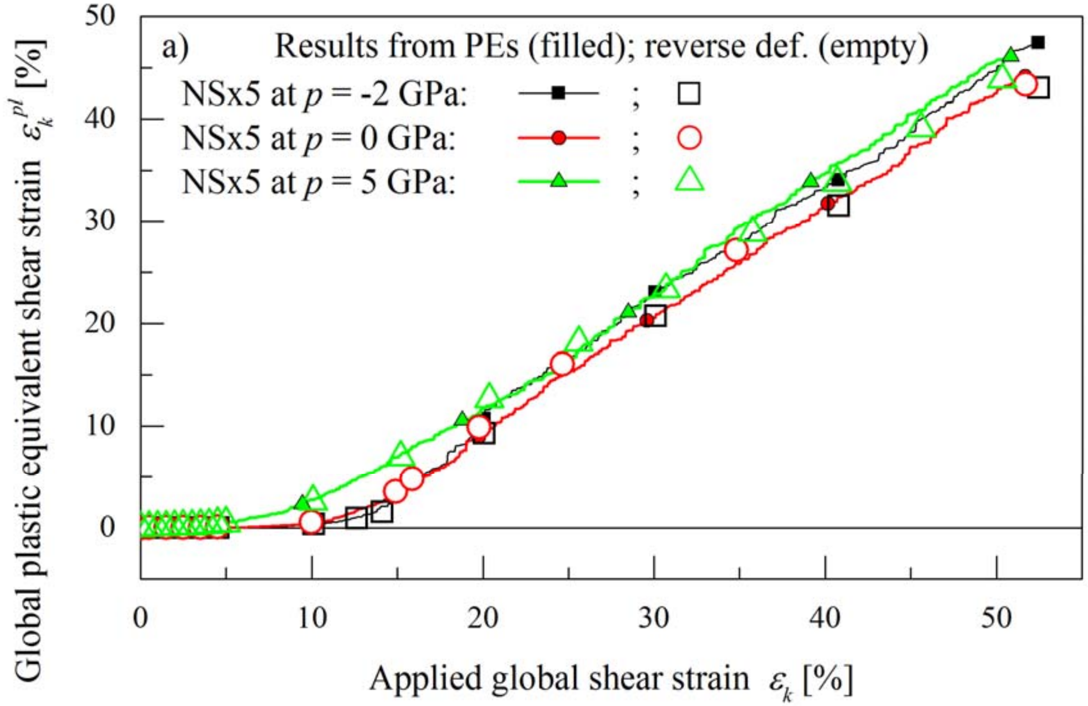


P. Y. Huang et al., Science, 2013.

G. Molnár et al., JNCS, 2016.
G. Molnár et al., PRE, 2017.

Atomistic response





$$d\underline{u}_{na} = d\underline{u} - d\underline{\underline{\varepsilon}} \cdot \underline{r}_0$$

Compression induces initial defects in the atomic structure which results in a quicker yielding

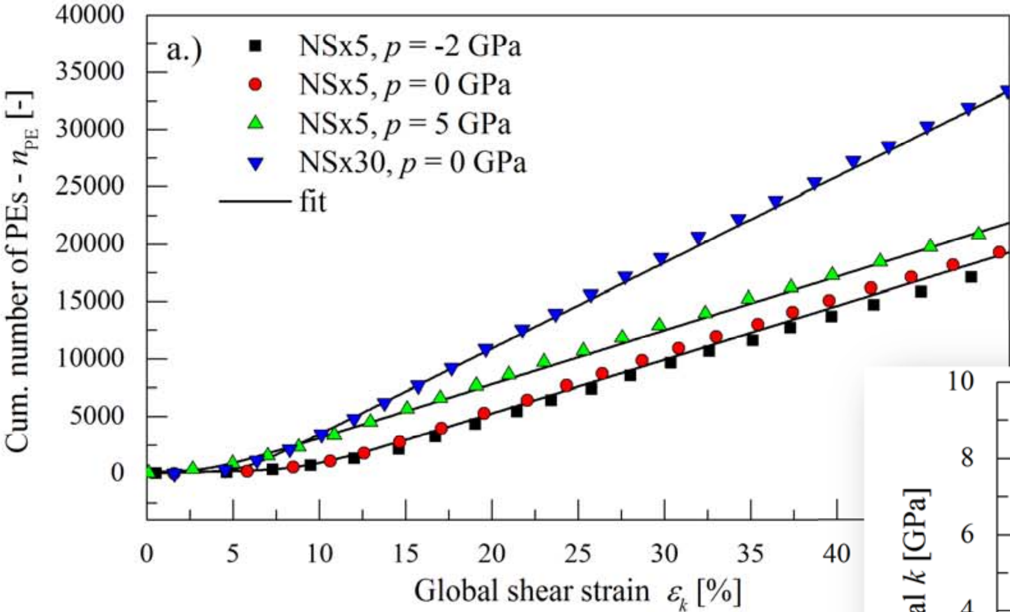
Plastic strain

$$\underline{\underline{\varepsilon}}^{pl} = \sum_{i=1}^{N} \frac{V^i}{V} \underline{\underline{\varepsilon}}^{PE,i}$$

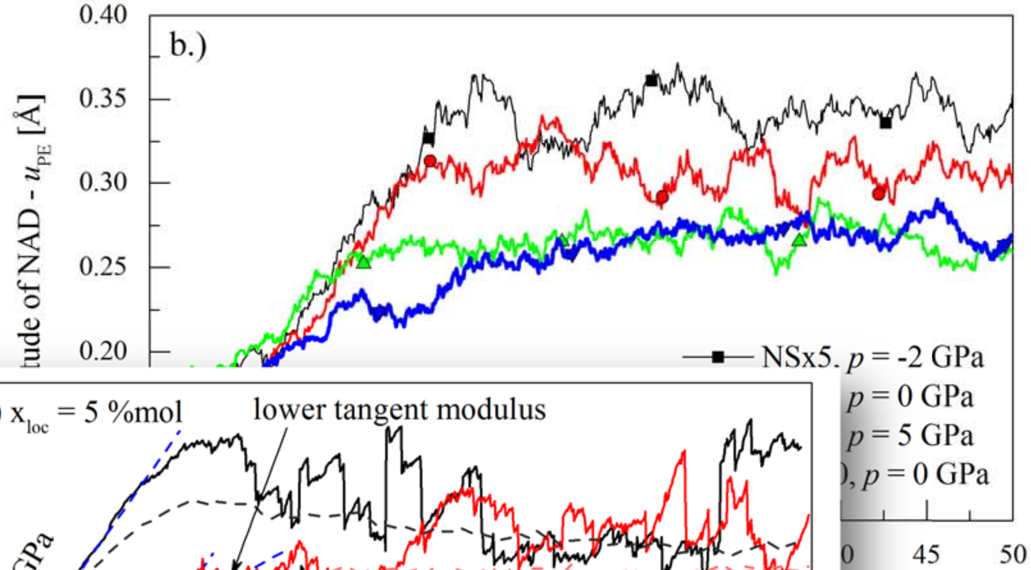
G. Molnár et al., JNCS, 2016.
G. Molnár et al., PRE, 2017.

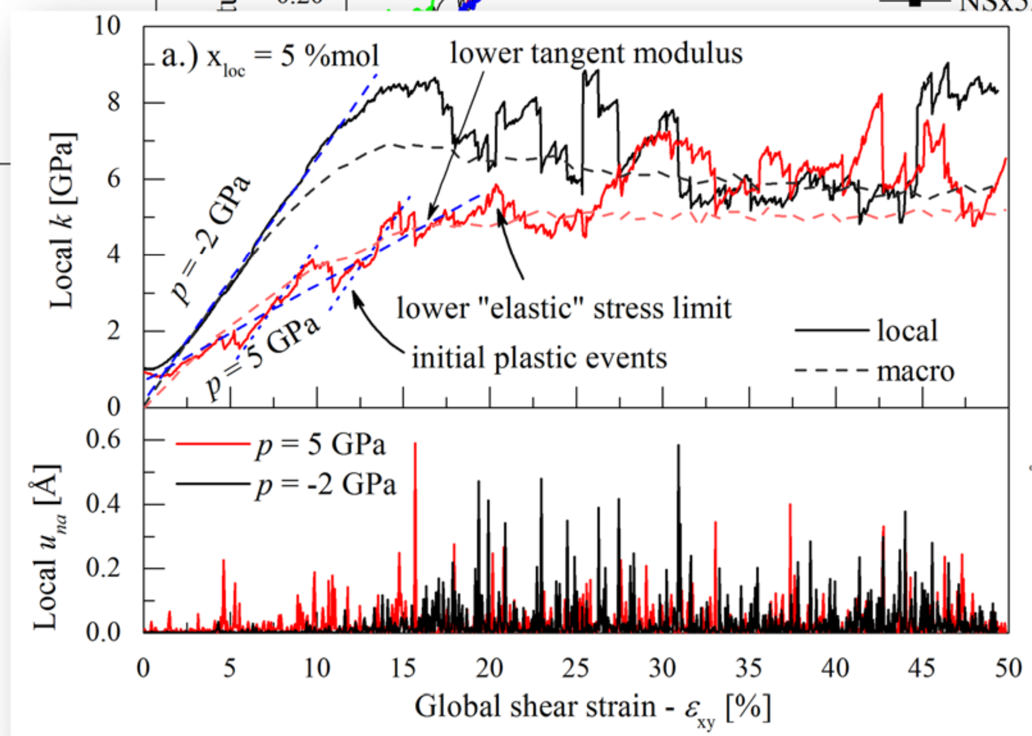
Atomistic response

Number of plastic events



Amplitude of plastic event



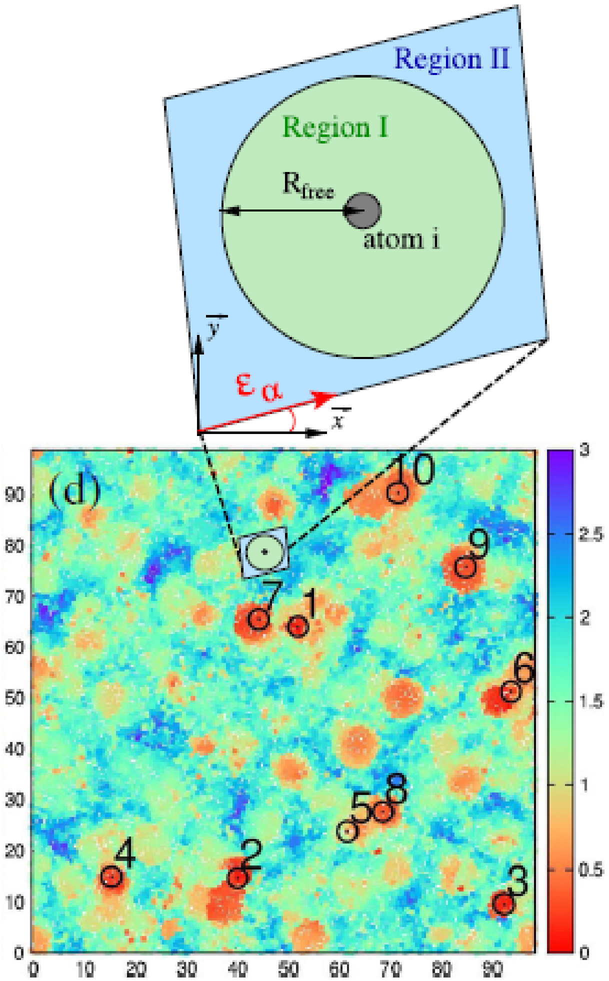


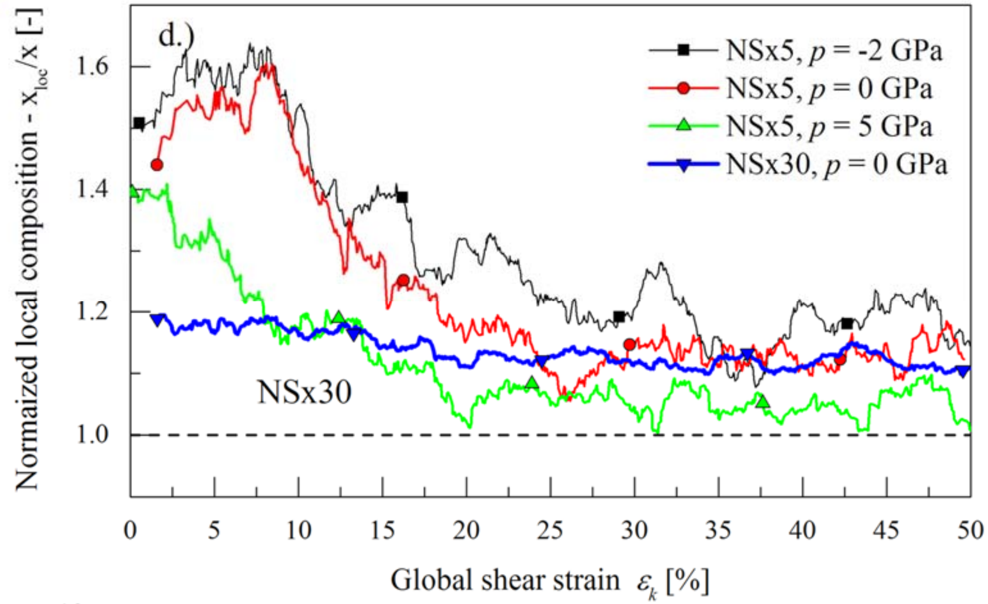
G. Molnár et al., JNCS, 2016.
G. Molnár et al., PRE, 2017.

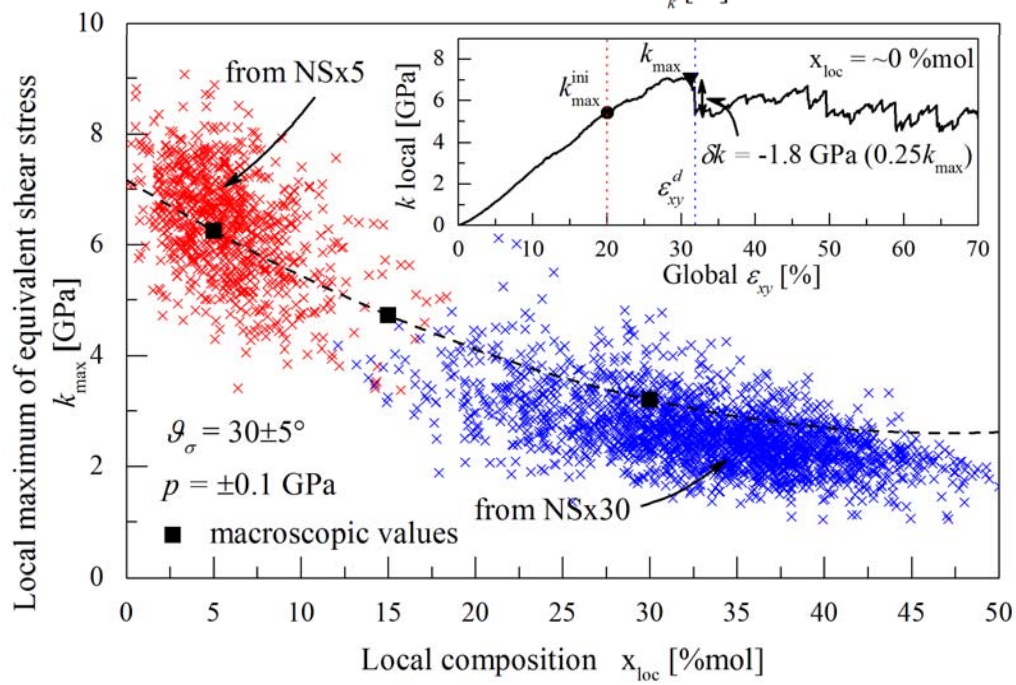
Atomistic response

Local strength vs local composition

S. Patinet et al., PRL, 2016.





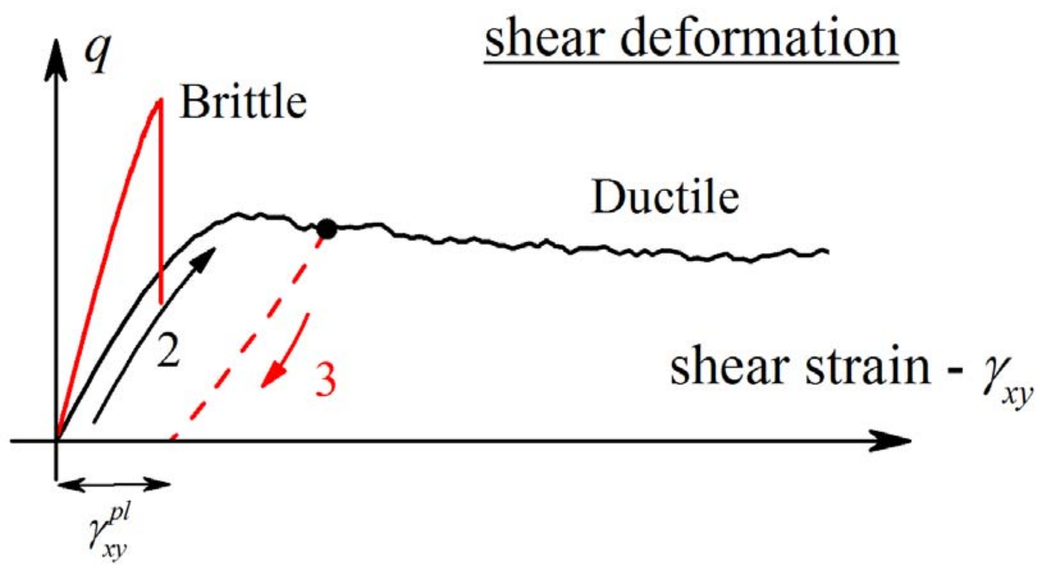


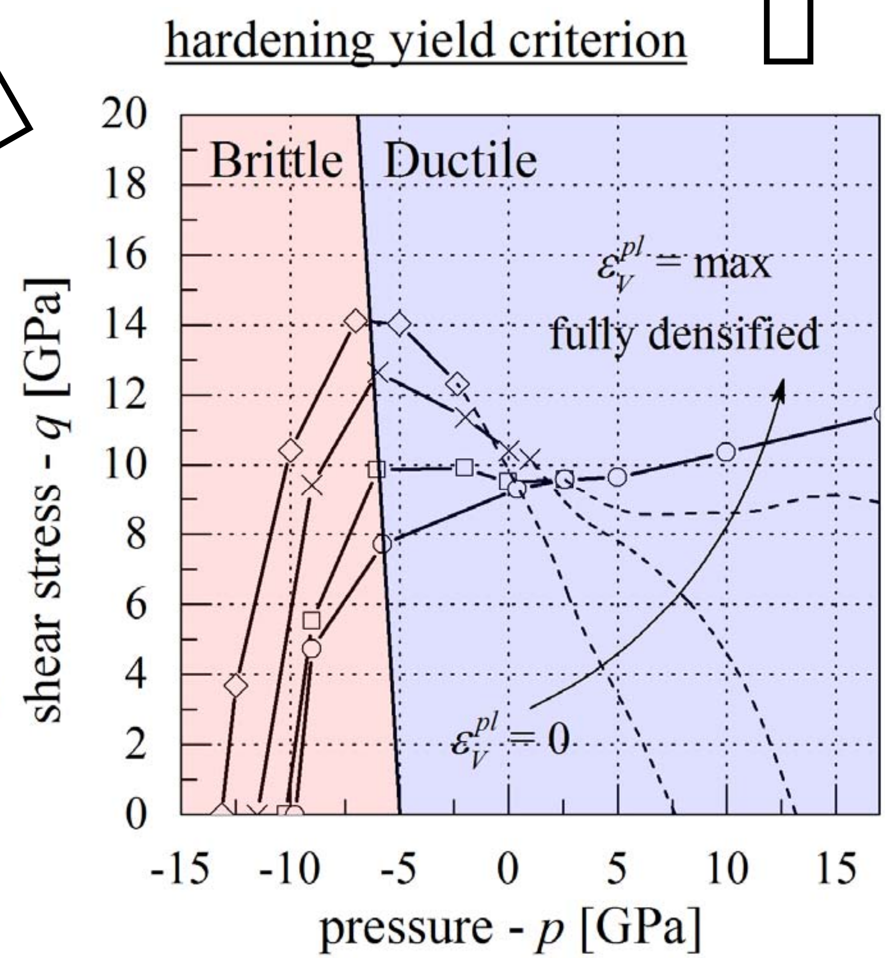
G. Molnár et al., MRS Advances, 2016

Atomistic response

Phase-field

Plastic material model





Different continuum treatment of brittle and ductile response

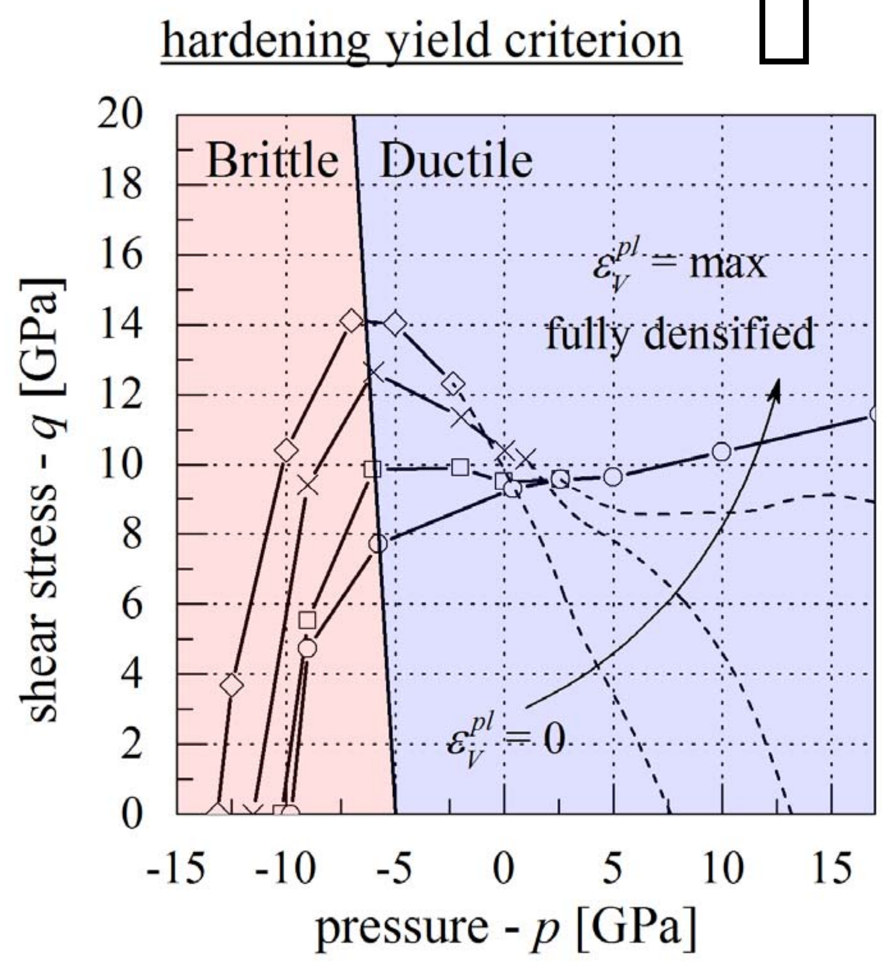
G. Molnár et al., MRS Advances, 2016

Atomistic response

Plastic material model

Calibration is necessary

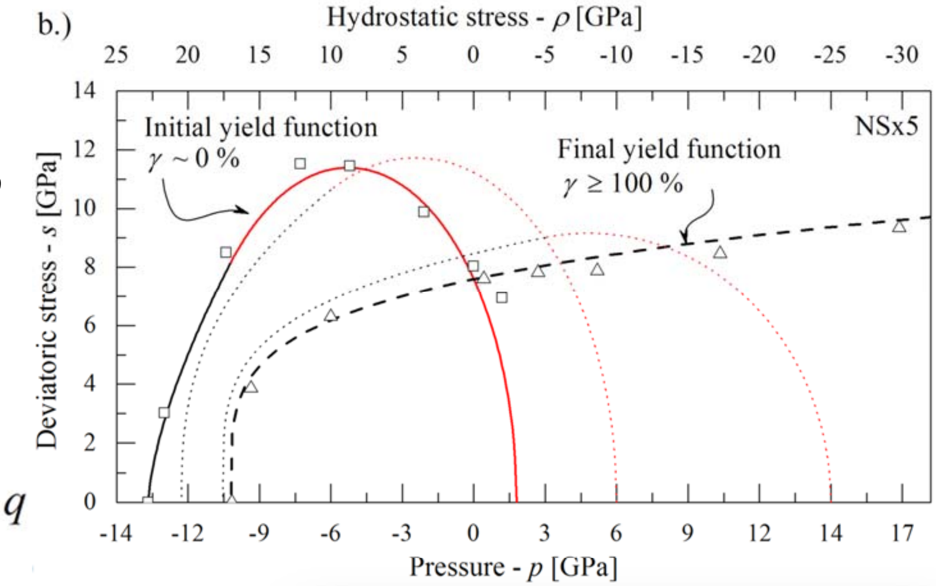
1. Real **temperatures**
2. Real **time**
3. **Surface** effects

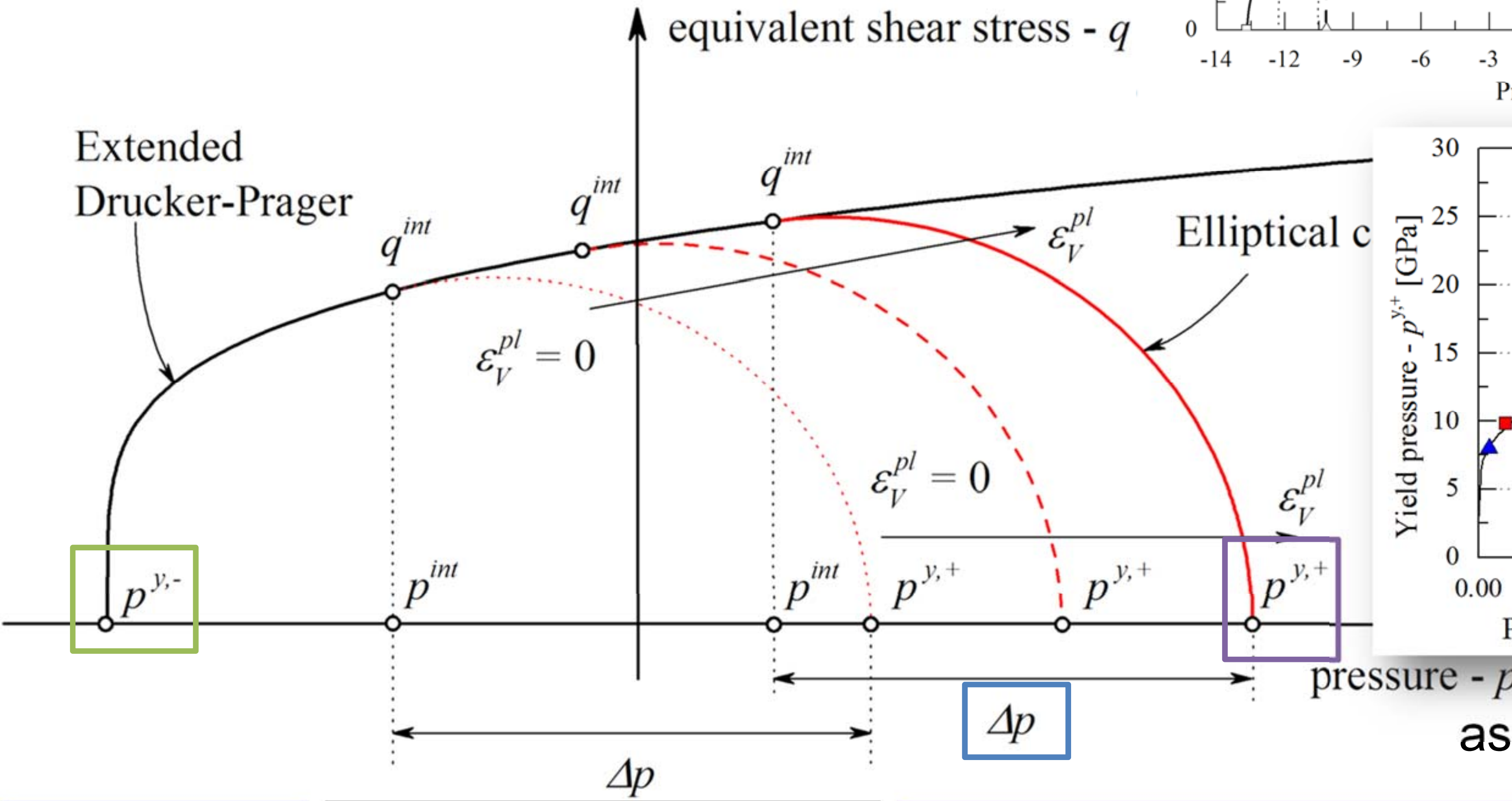


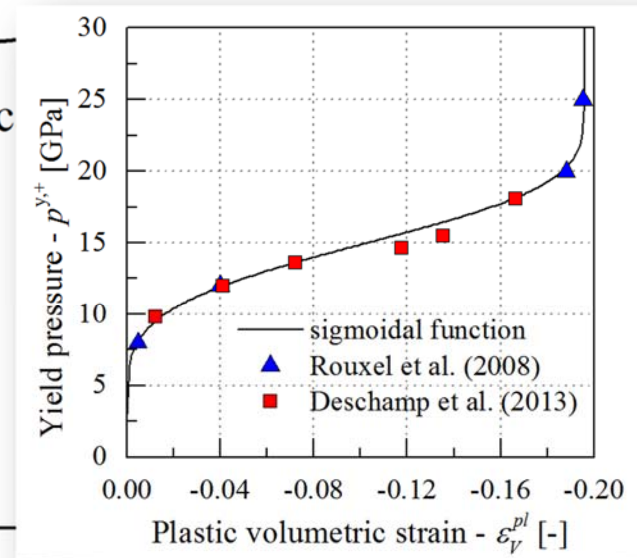
G. Molnár et al., Acta Materialia, 2016.
G. Molnár et al., Mech of Mat., 2017

Yield criteria

$$F = \begin{cases} \left(\dfrac{q}{c}\right)^{b} + \dfrac{p^{y,-} - p}{a} = 0 & \text{if} \quad p^{\text{int}}\left(\varepsilon_V^{pl}\right) \geq p \\ \left(\dfrac{p - h\left(\varepsilon_V^{pl}\right)}{d\left(\varepsilon_V^{pl}\right)}\right)^2 + \left(\dfrac{q}{e\left(\varepsilon_V^{pl}\right)}\right)^2 - 1 = 0 & \text{otherwise,} \end{cases}$$



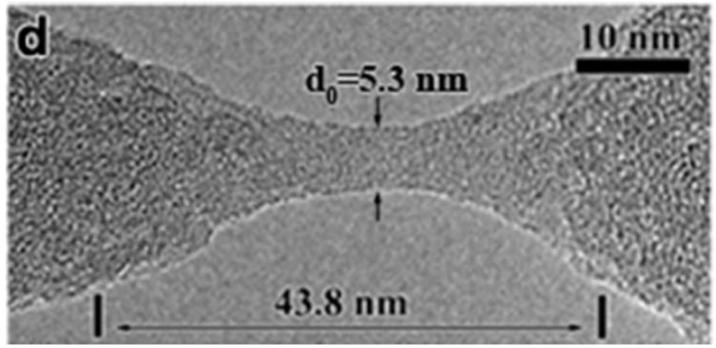


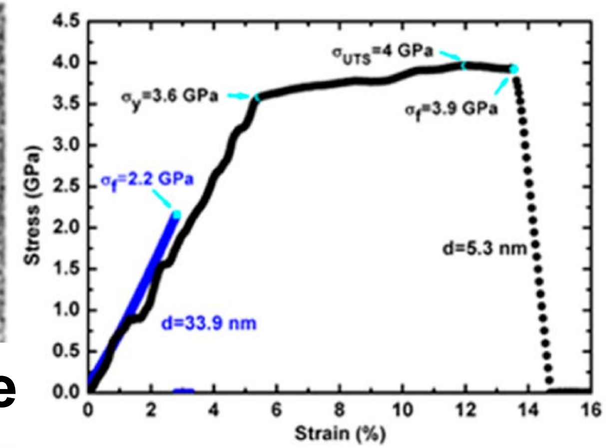


associated flow rule

Luo et al., Nano Lett., 2014.

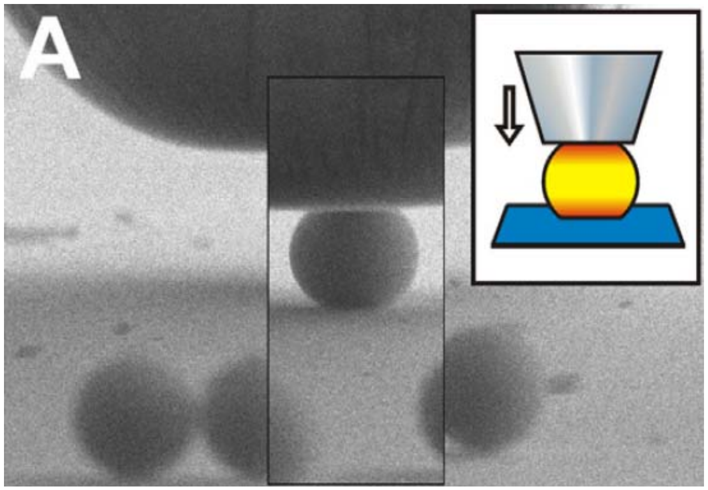
Calibration

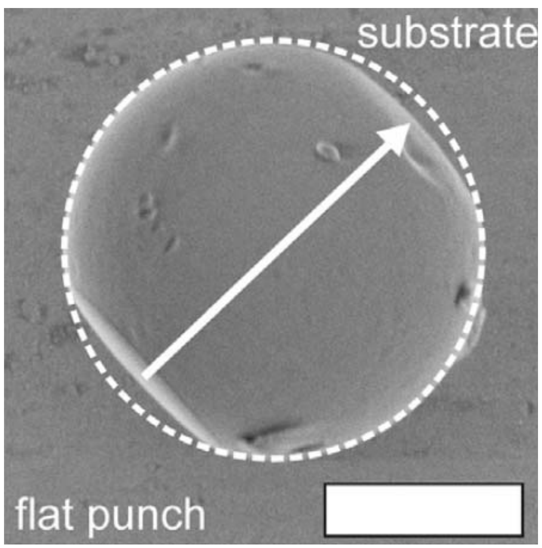


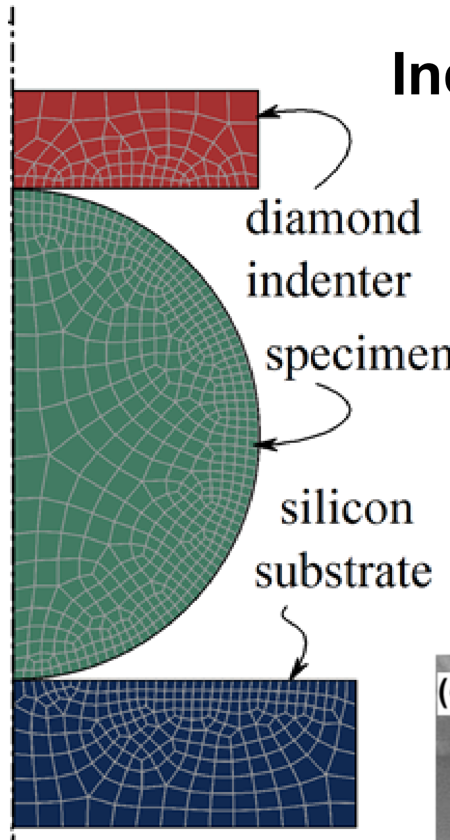


Nano-wire

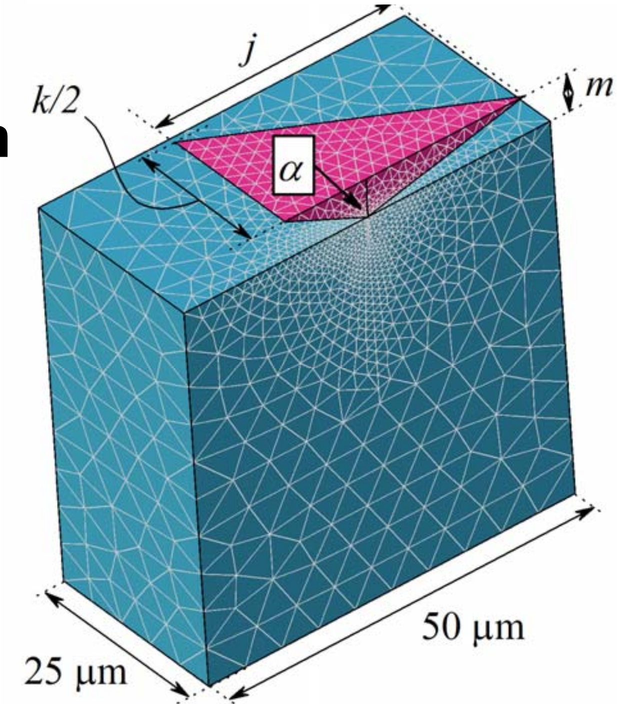
Micro-sphere

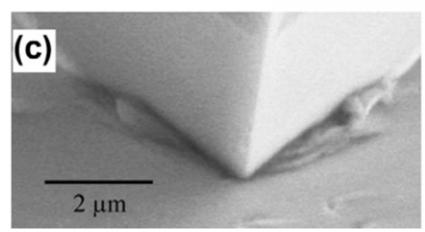


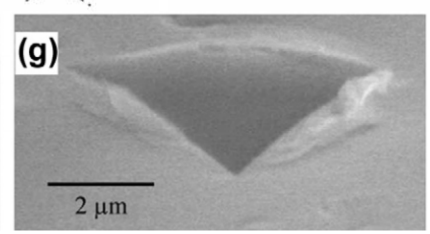




Indentation





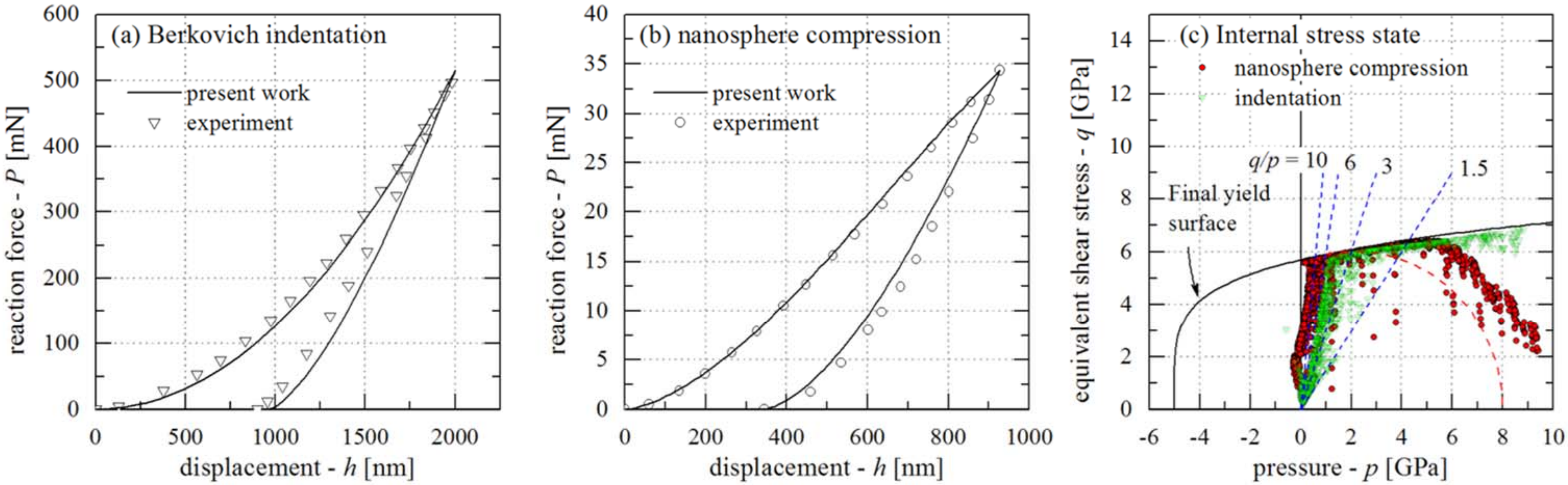


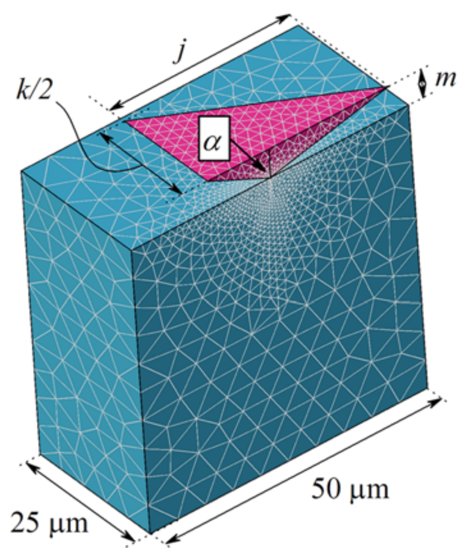
S. Romeis et al., SM, 2015.

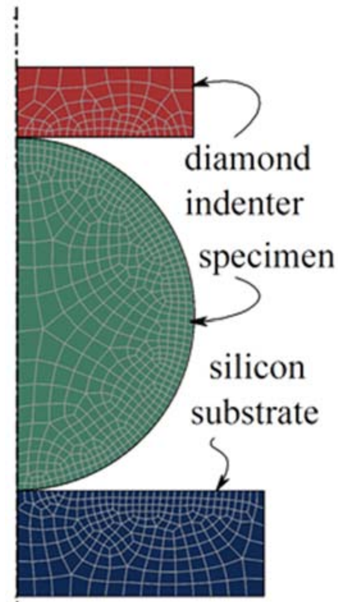
H. Nili et al., PMS, 2013.

G. Molnár et al., Mech of Mat., 2017

Calibration

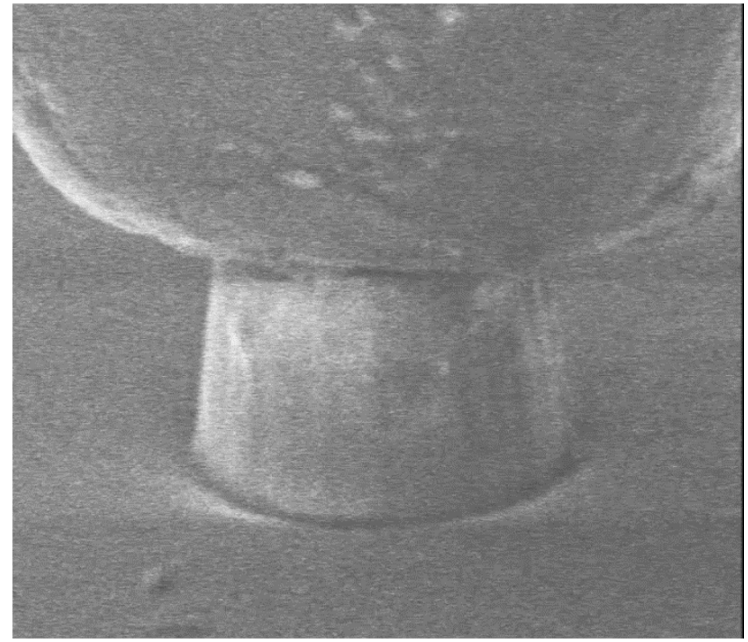






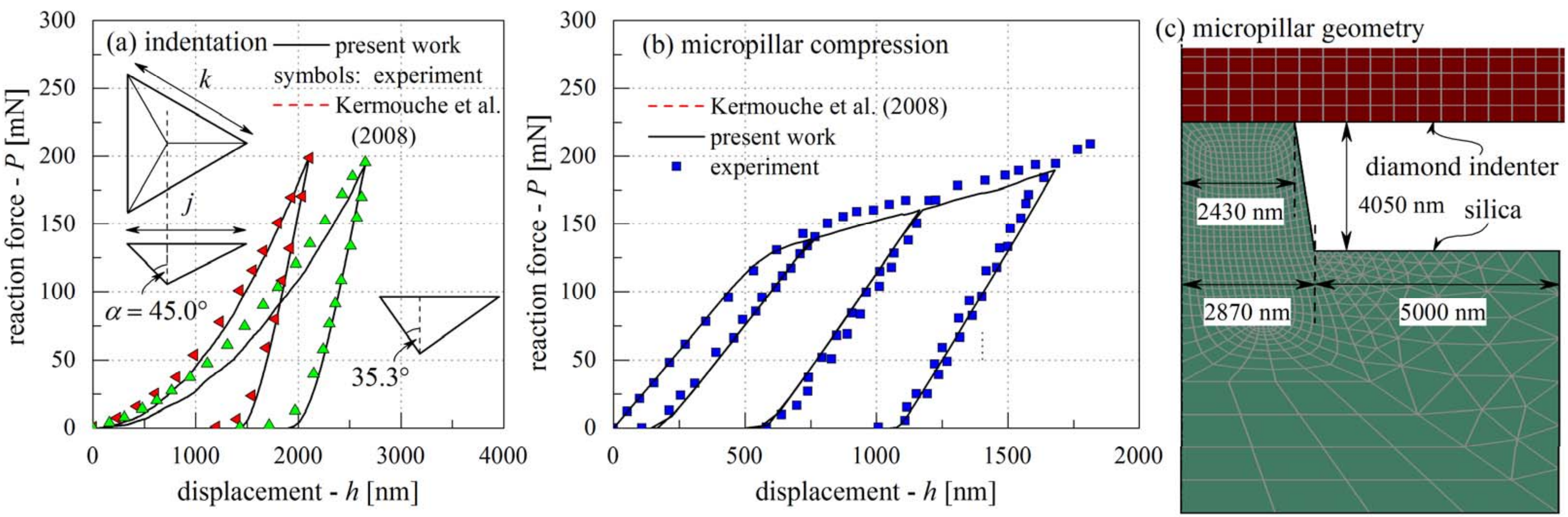
Verification

Room temperature
Real life loading rate
Micrometer size



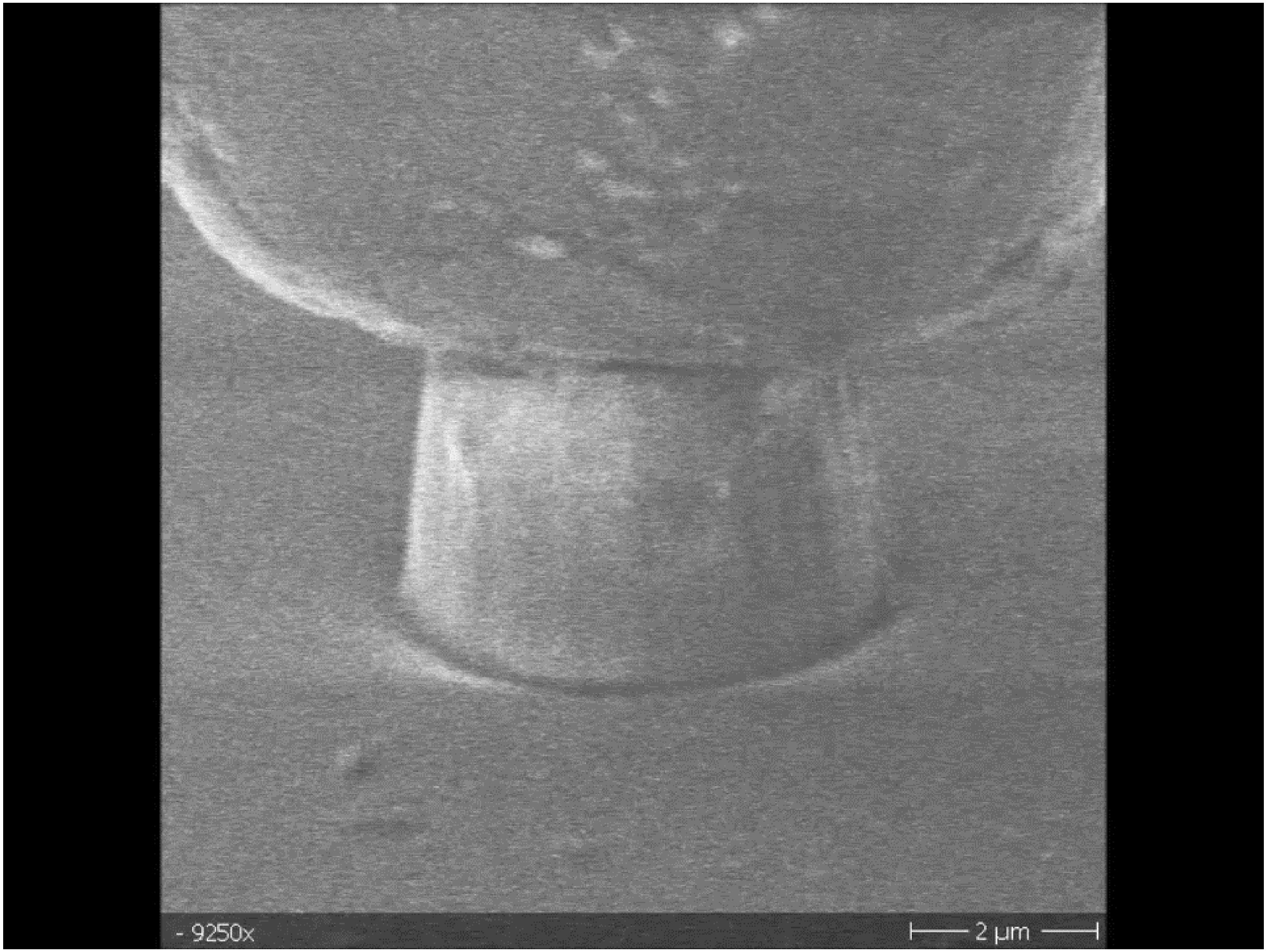
Indentation

Pillar

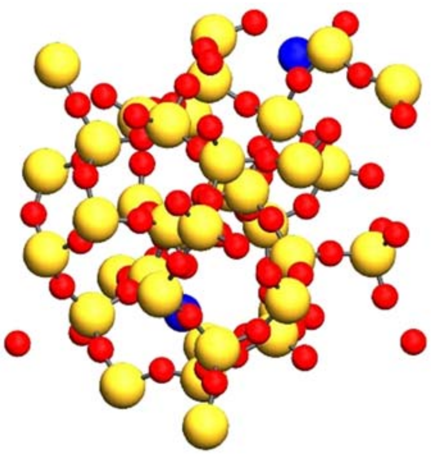


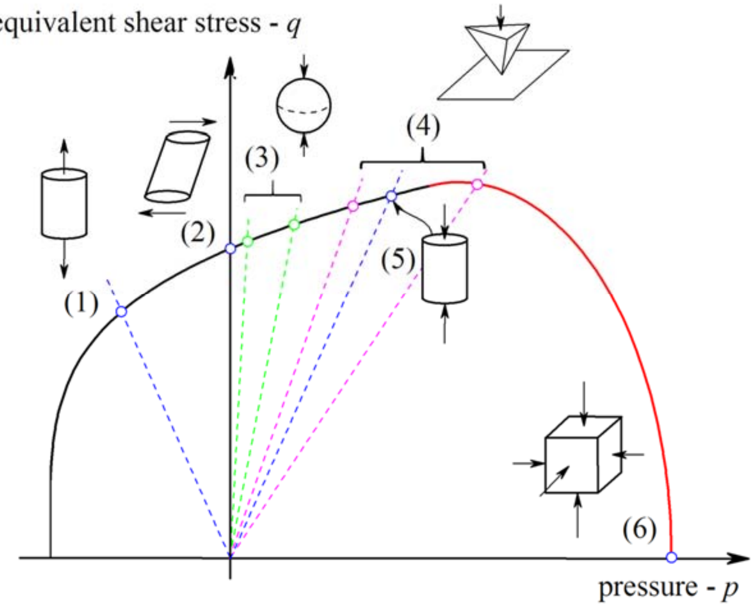
Verification

G. Kermouche et al., AM, 2016.



Conclusion





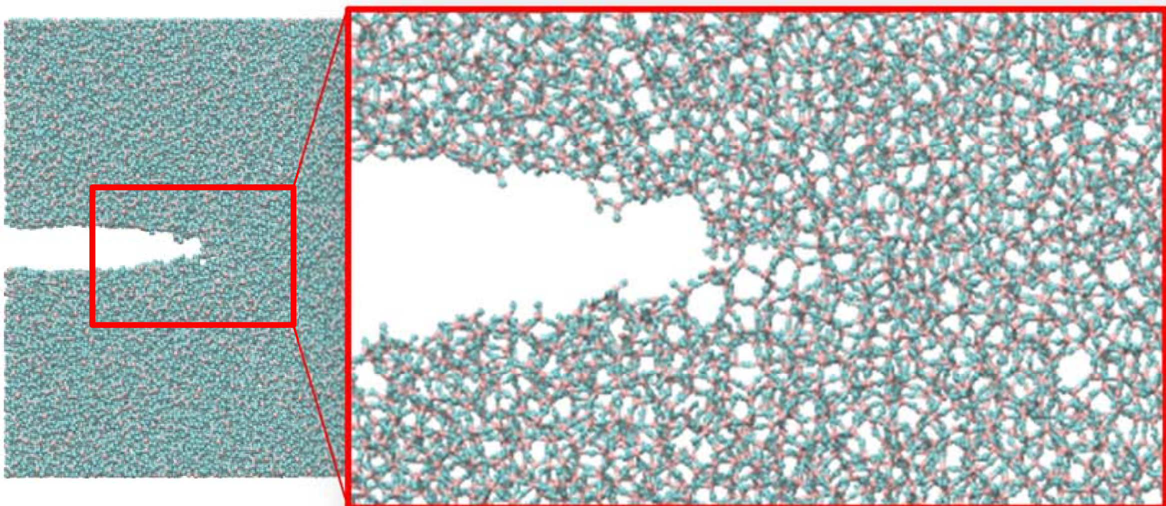
1. **Constitutive** model from **atomic scale** simulations
2. **Elementary mechanism** responsible for glass plasticity
3. Good **experimental correspondence**

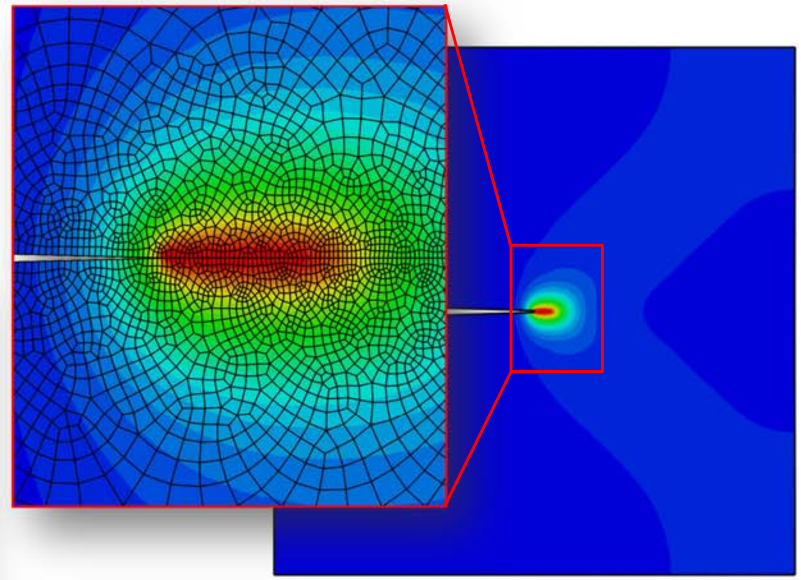
Outlook

Modeling brittle fracture

(in collab. with Anthony Gravouil, INSA)

Diffused damage → **Phase-field method**





Open source implementation of **ABAQUS/UEL**

MORE: www.molnar-research.com
(Examples, tutorial, theory)

&

GDR MÉPHY

27-28th of November, 2017

Gergely Molnár
gmolnar.work@gmail.com
www.molnar-research.com