DENSIFICATION OF FUSED SILICA BY STRESS OR LASER IRRADIATION

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3rd Int'l Workshop on Flow/Fracture of Advanced Glasses

Penn State, October 2005

OUTLINE

- REVIEW
- Densification expts via pressure
- Surface response: Grinding & Polishing
- Indentation (microscopy, SEM, Raman)
- MD simulations

- CONSTITUTIVE LAW: Yield function, flow potential, hardening

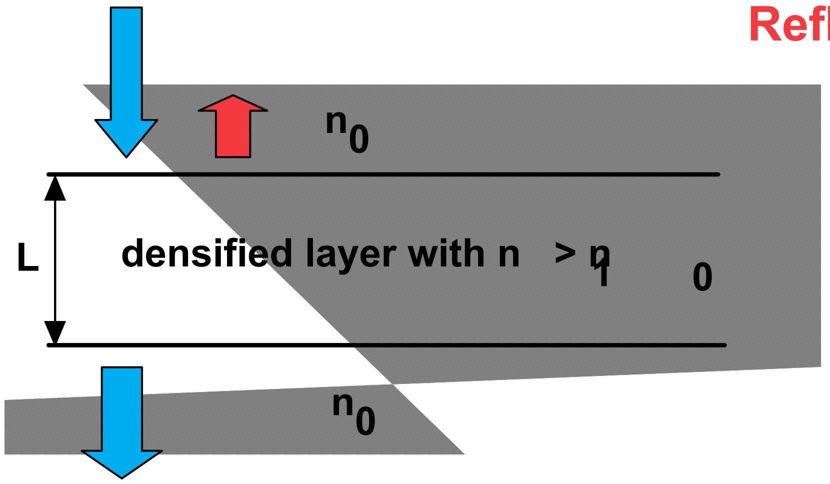
- FEM RESULTS: Axisymmetric, Berkovich, Vickers, Knoop

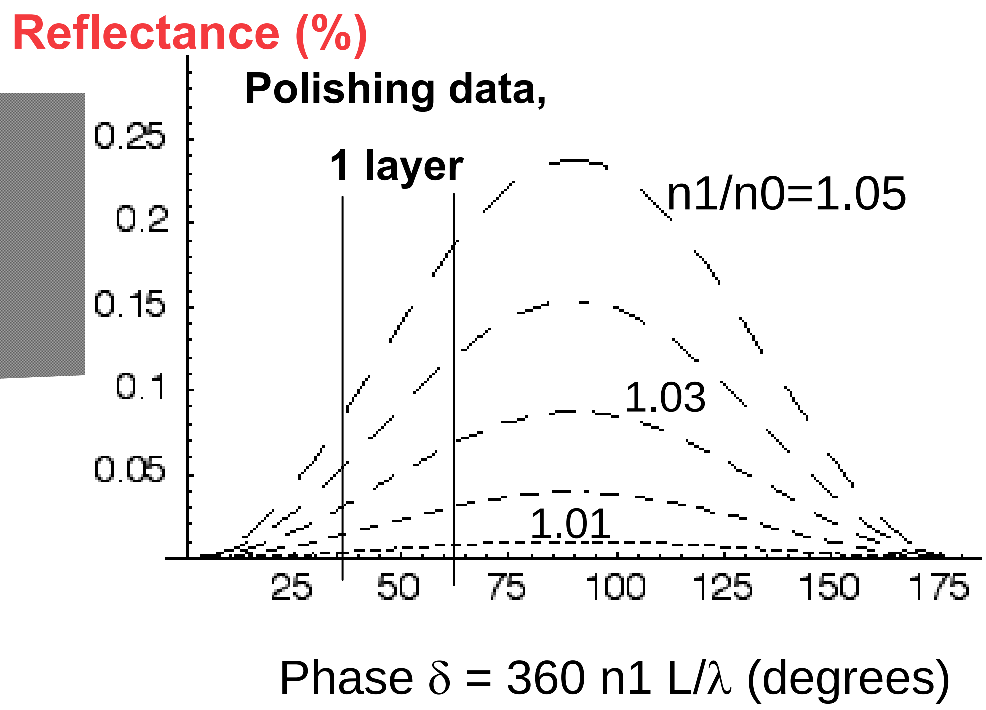
- MD SIMULATIONS: laser-induced densification
- Fluence, pulse duration, elastic moduli

POLISHING OF FUSED SILICA & IMPLICATIONS (Yokota et al., 1969; Malin & Vedam, 1977)

Ellipsometric measurement of index of refraction

$\Delta n/n \leq 5\%$; Layer thickness 20-70 nm



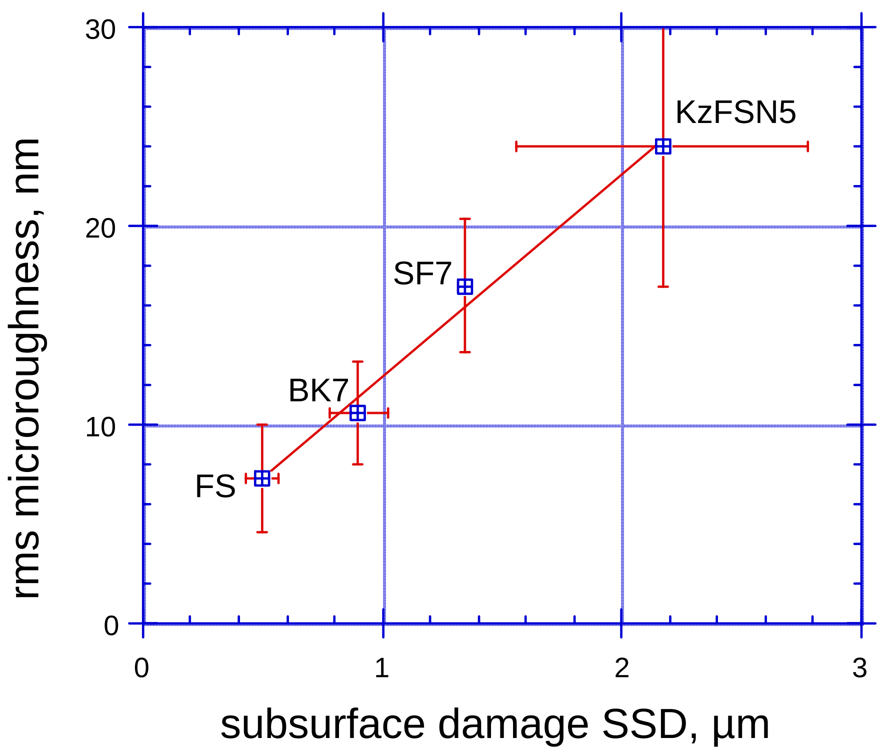


DETERMINISTIC MICROGRINDING(Rochester, 1993-98)

2-4 µm bound diamond abrasive tool

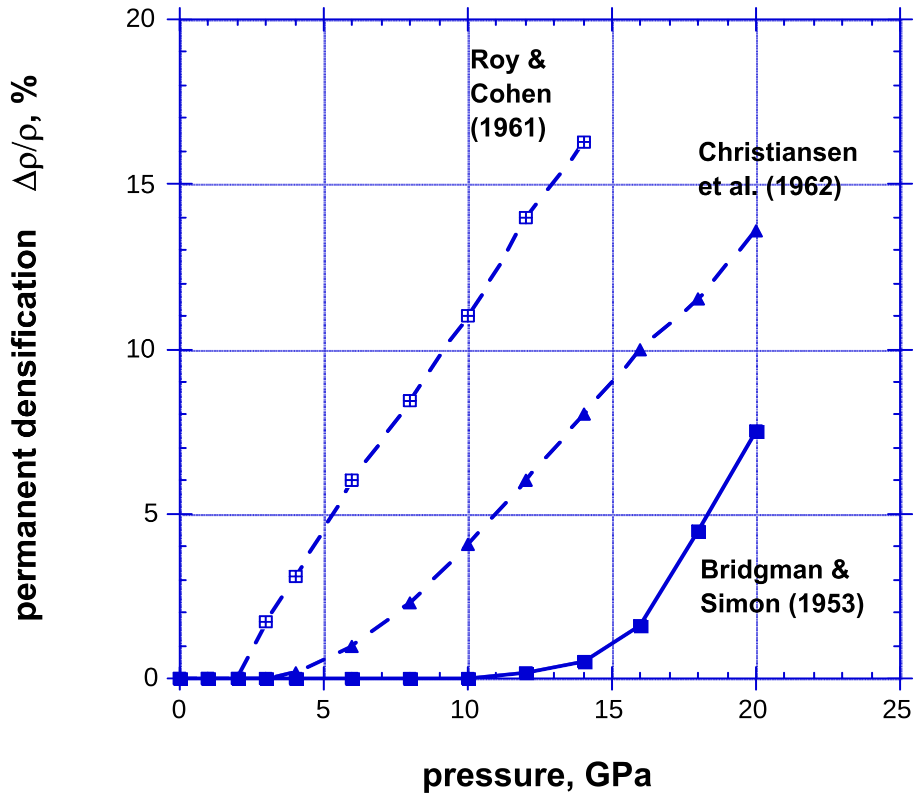
Infeed rate ~ 6 µm/min

FS produces superior finish, minimal subsurface damage



PERMANENT DENSIFICATION
Effects of pressure (and shear)

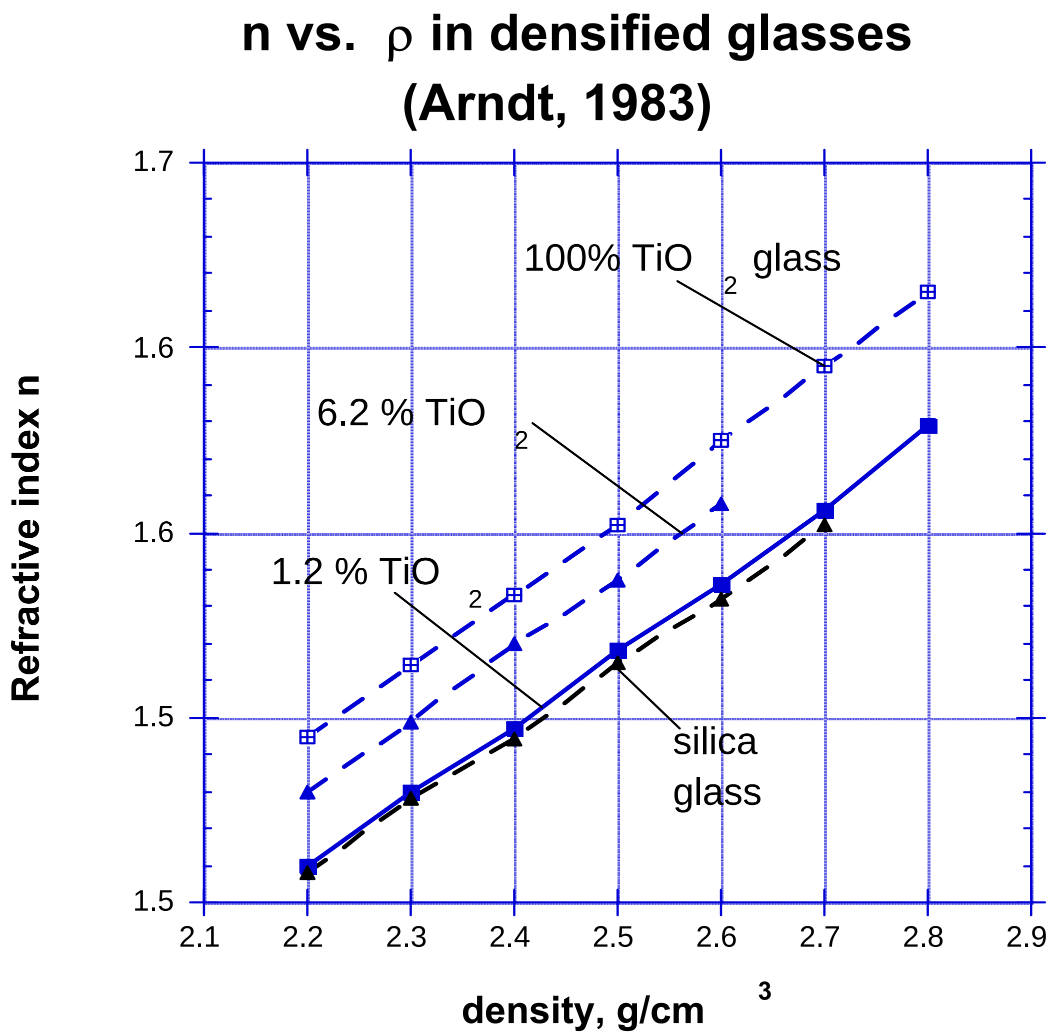
Permanent densification of fused silica @ 25 °C °C



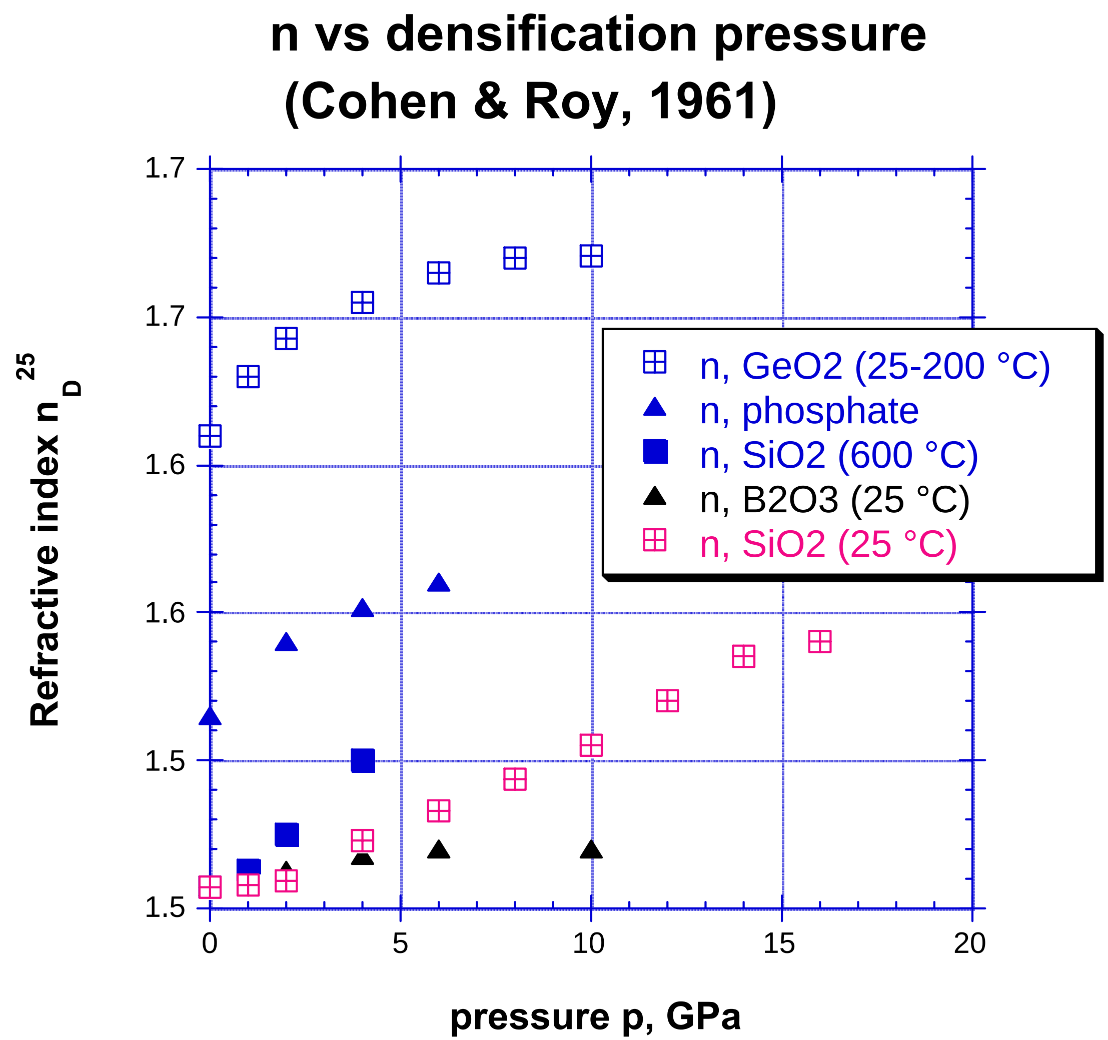
Pressure transmitting medium in high pressure cell:

Al2O3 (high shear) vs AgCl (low shear)

EFFECT OF DENSIFICATION ON n: $\Delta n/\Delta\rho$ ~ 0.025 1/(g/cc)

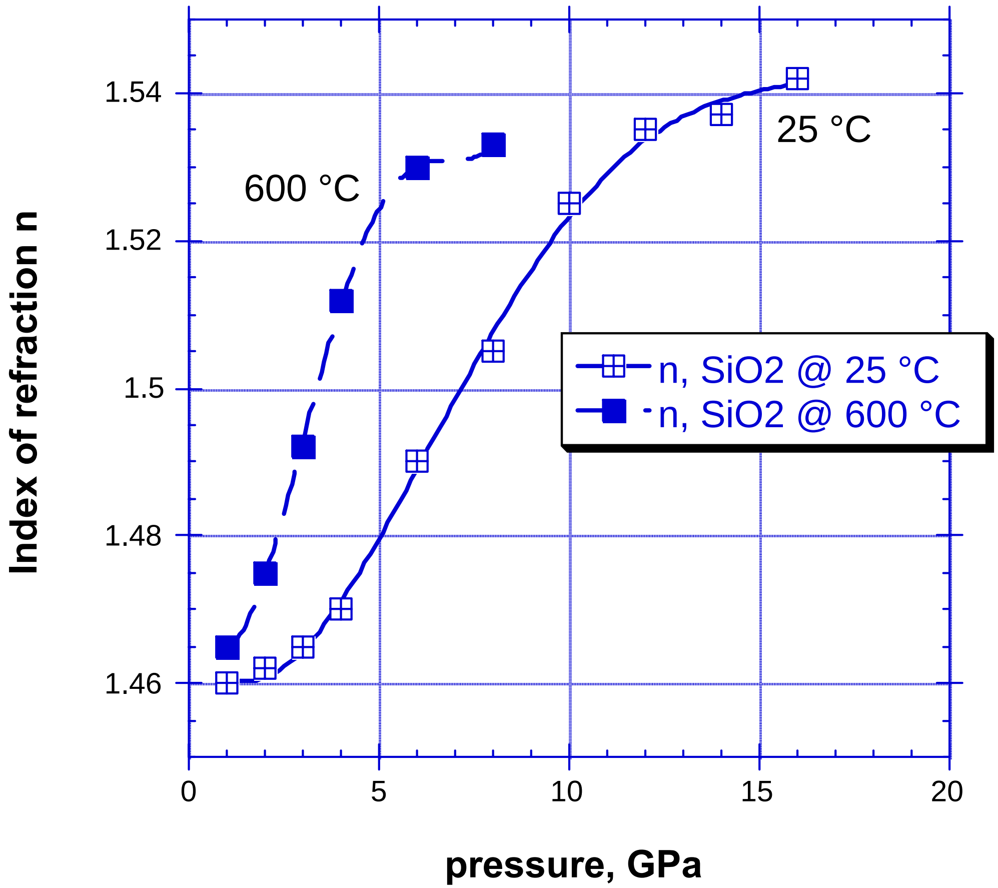


Different glasses densify: n vs pressure



Densification of SiO2 shows saturation and thermal activation (Cohen & Roy, 1965)

Effect of pressure & temperature on densification

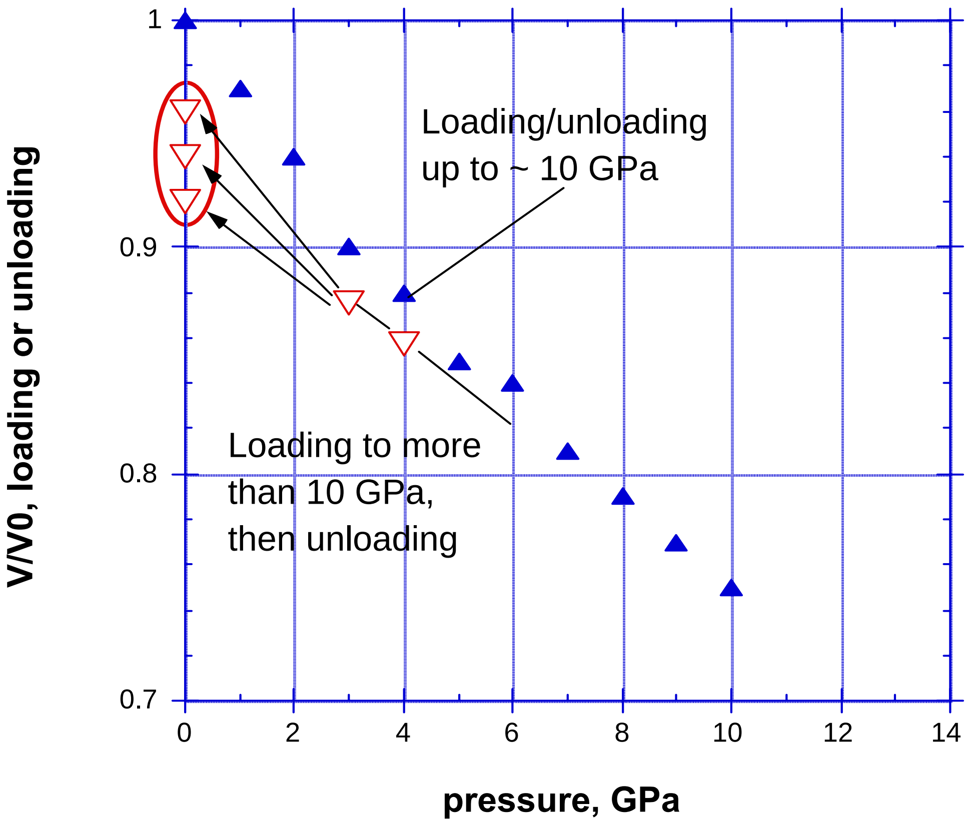


Volume strain vs pressure in fused SiO2 (Meade & Jeanloz, 1987)

In situ measurements; diamond cell; scribed grid on sample

4:1 mixture of MeOH-EtOH;

pressure is hydrostatic up to (at least) 10 GPa



Vickers indentation in quartz, soda-lime glass, FS at RT or at 77 K (Kurkjian et al., 1995)

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QUARTZ: plastic flow by shear @ RT and @ 77 K

SODA-LIME GLASS: plastic flow by shear @ RT, densifies @ 77 K

FUSED SILICA: densifies both @ RT and @ 77 K

Topography of indentation in densified glass:

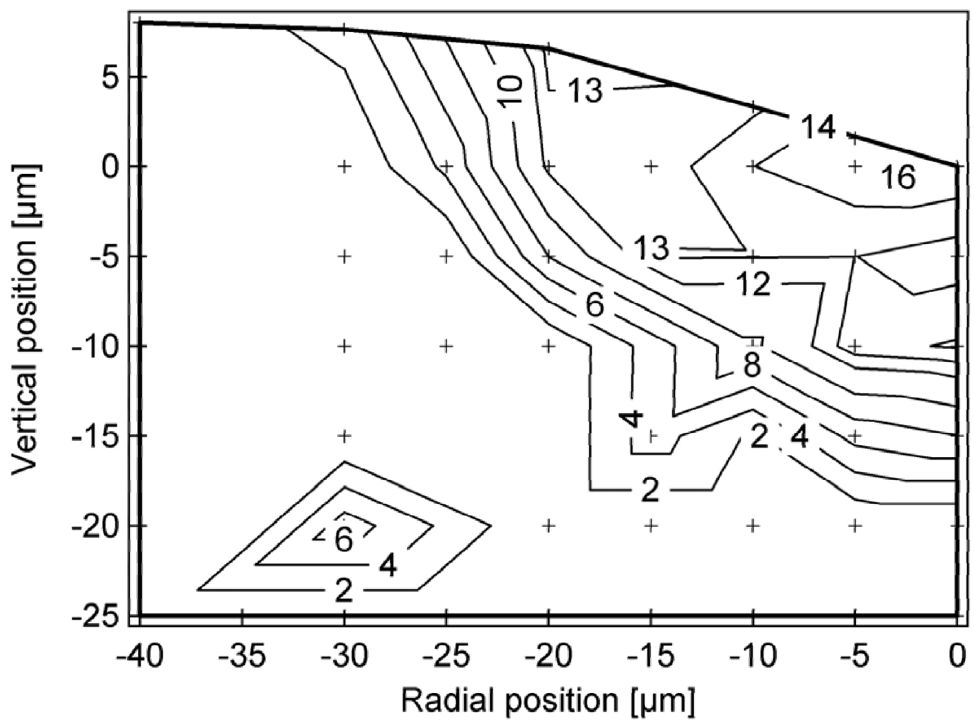
Absence of shear flow lines,

Absence of pile up around indent edge

Raman micro-spectroscopy (Perriot et al., 2005)

Iso-densification lines for Δρ/ρ0 (%) under indent :

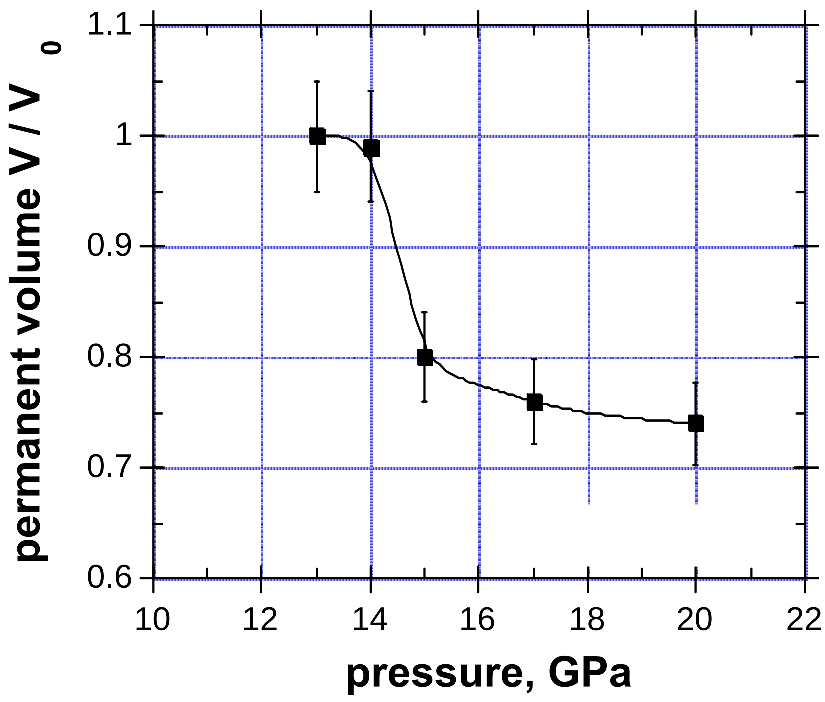
Densification from 2-16 %



MD simulation in amorphous SiO2 @ RT (Tse, 1992)

Si coordination number increases from 4 to ~ 6

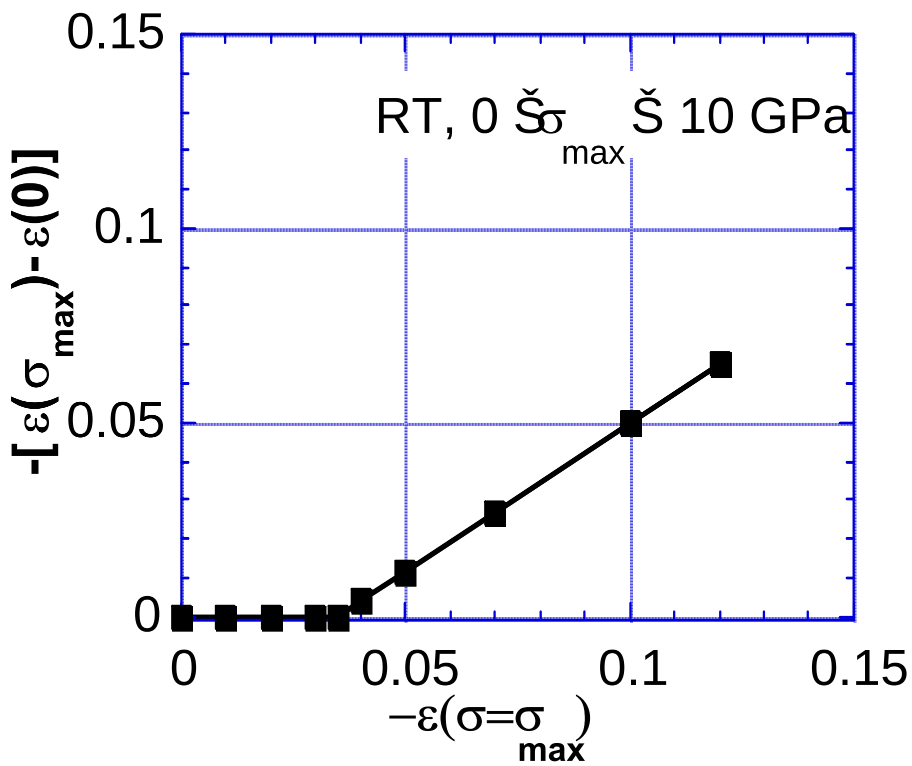
as permanent volume V decreases from V0 to ~0.75 V0



MD of uniaxial compression (Vogel et al., 1996)

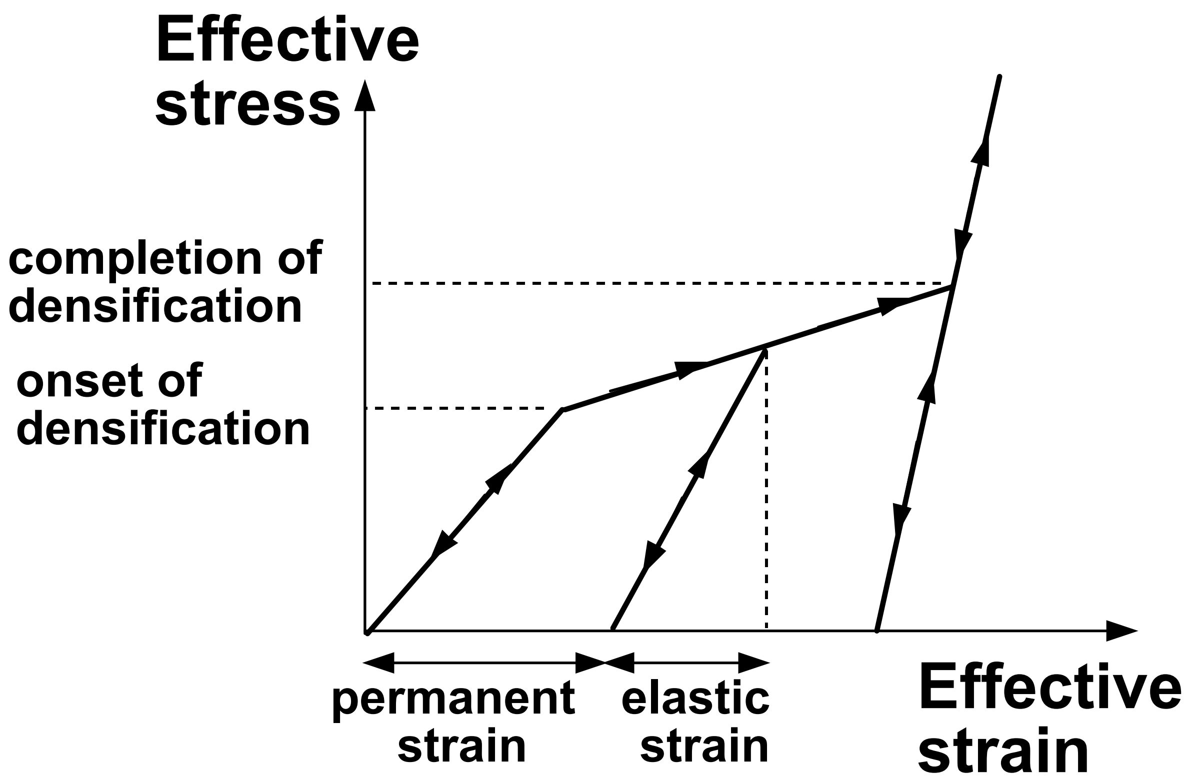
Plastic (i.e. permanent) strain vs. total strain (i.e. max load)

"Permanent strain"



"max load"

CONSTITUTIVE LAW: Stress-strain curve

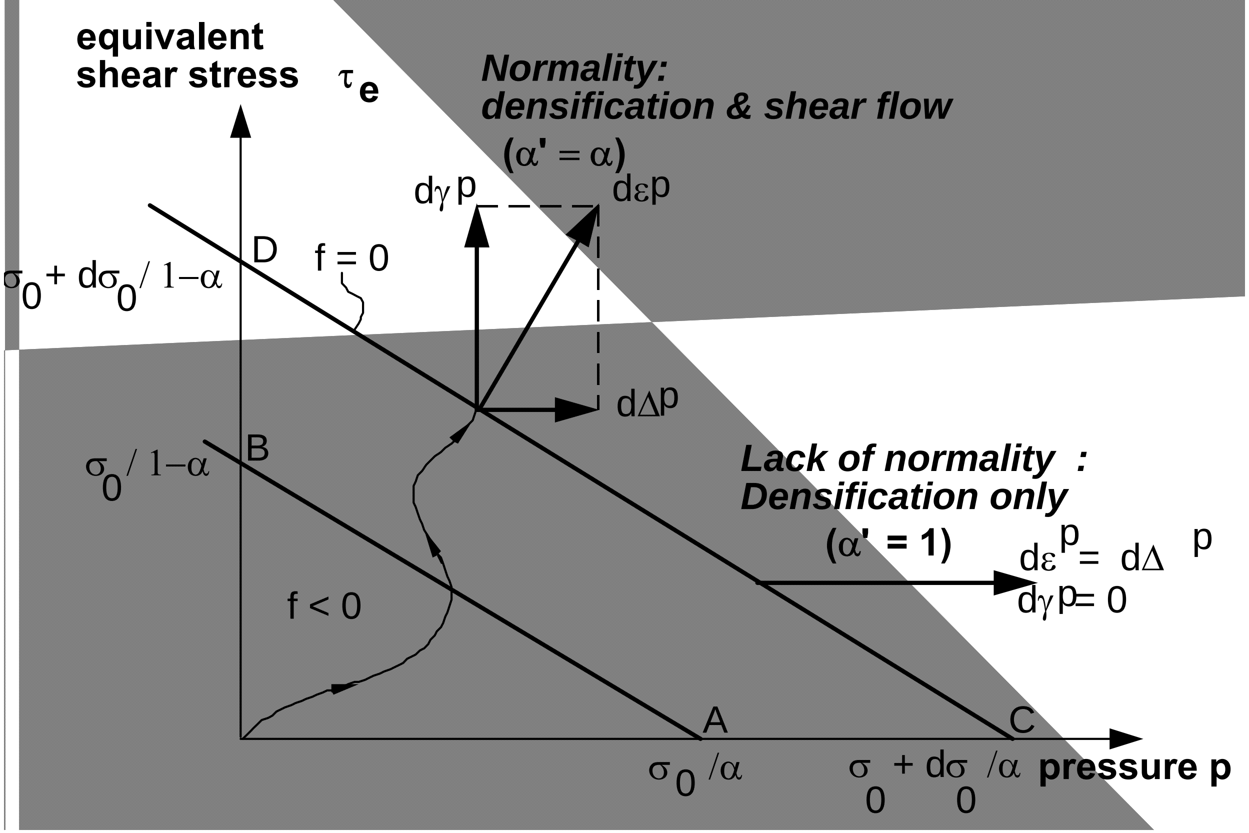


CONSTITUTIVE LAW: FLOW RULE & HARDENING
hardening modulus h = 14 - 32 GPa

σ_0 ~ "yield stress"

α ~ effect of pressure on yield stress

α' ~ contribution of densification to total deformation



DENSIFICATION OF FUSED SILICA BY STRESS OR LASER IRRADIATION
Part 2

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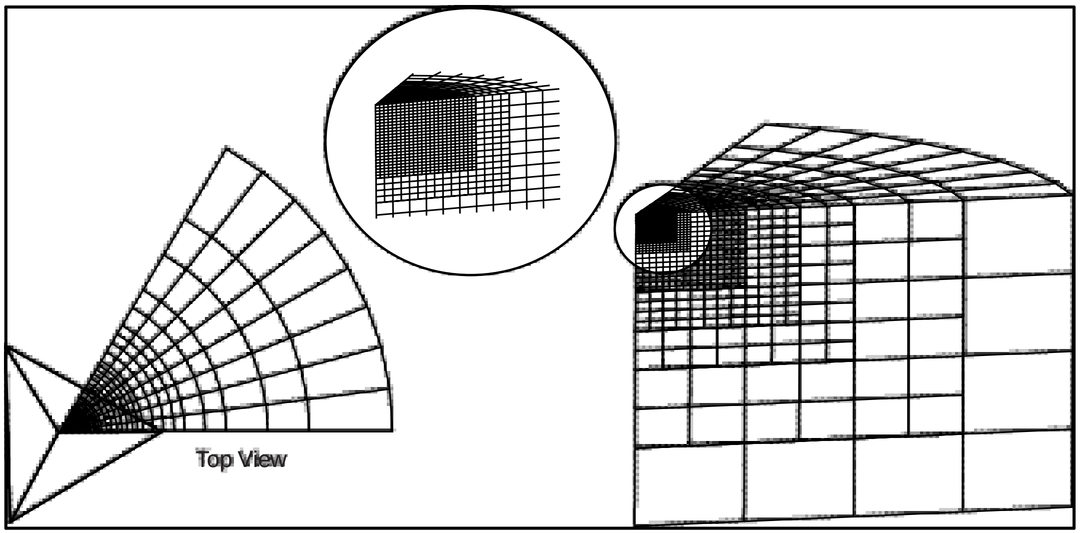
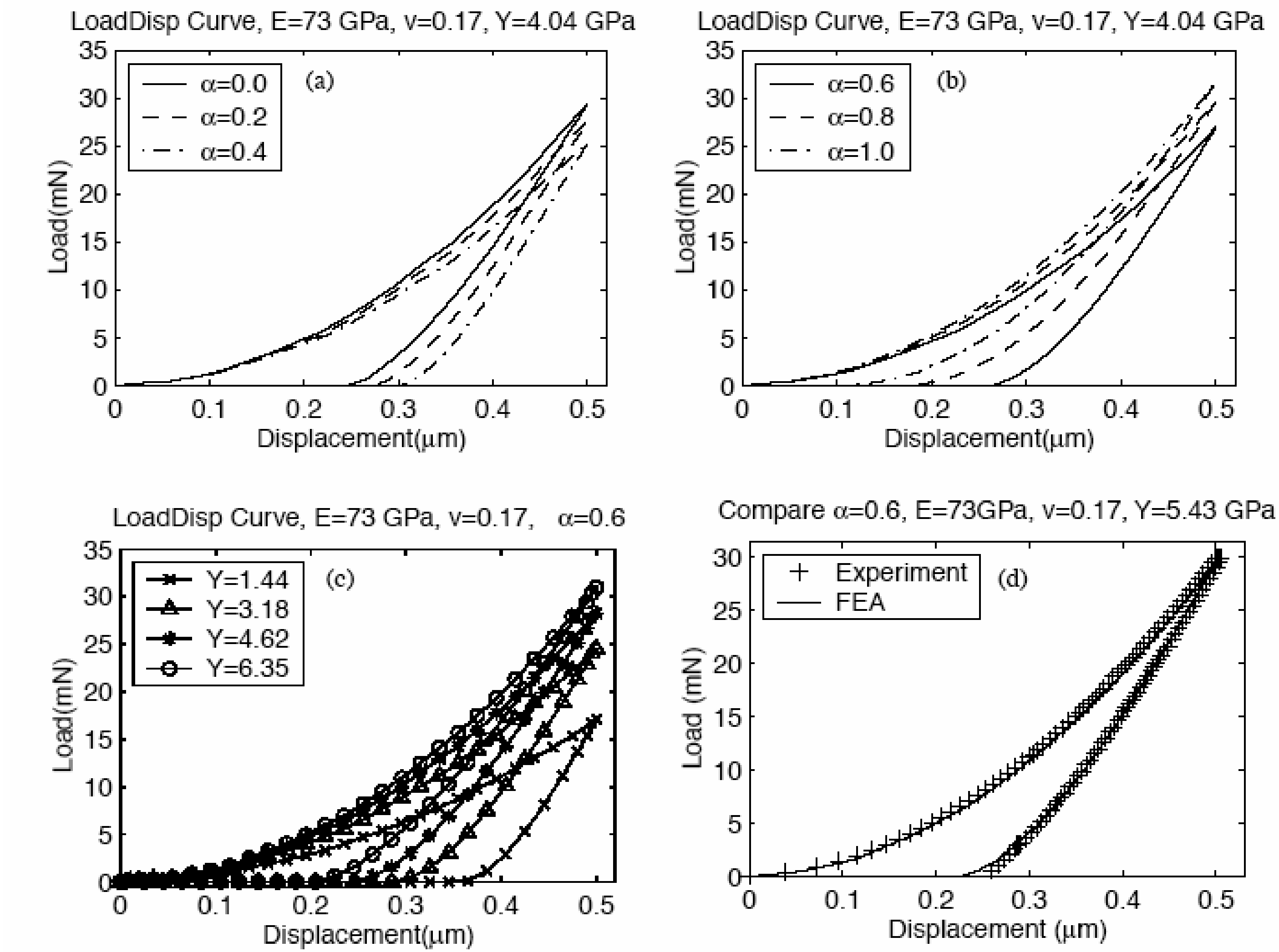
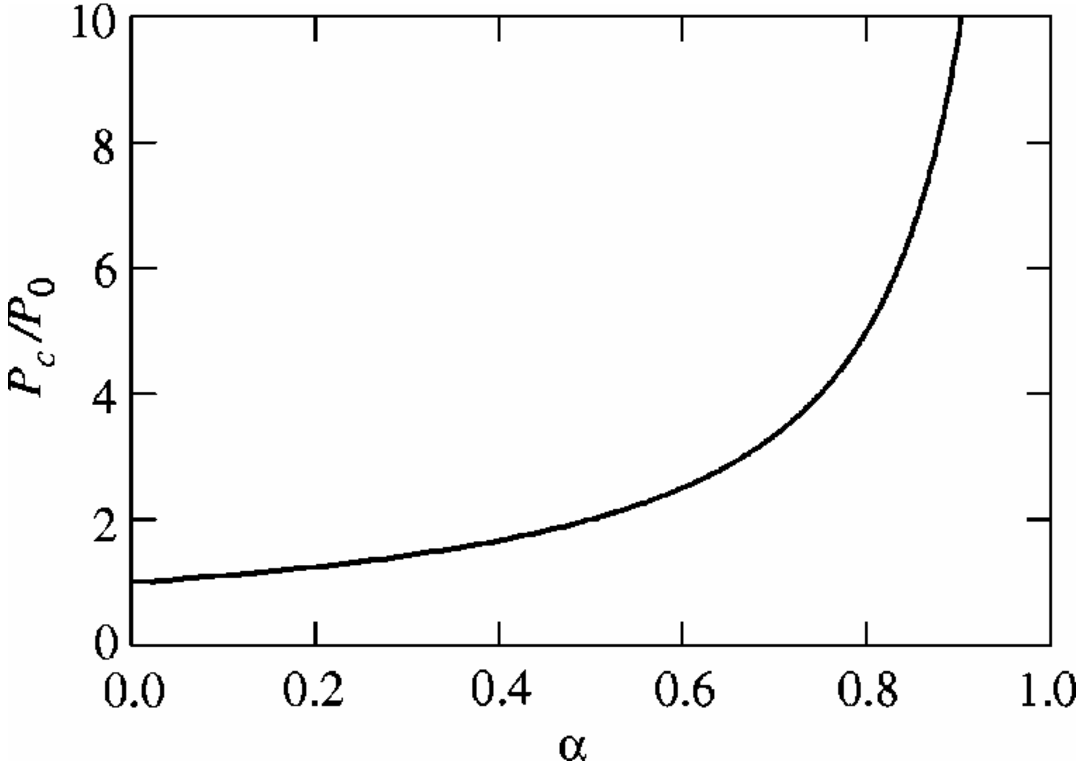
FEM analysis: 3D, Berkovich tip



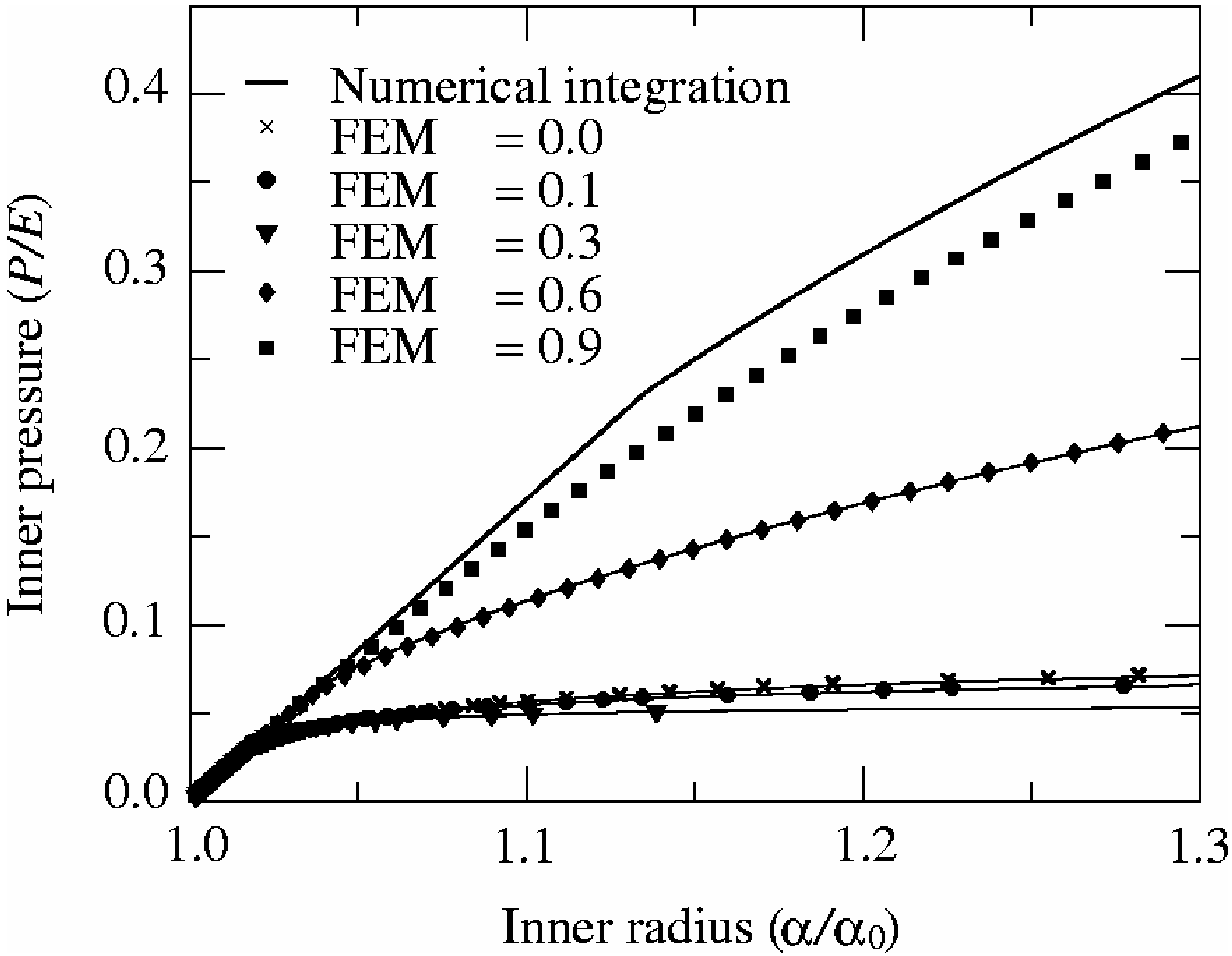
FEM analysis: Effect of densification parameter α & comparison with nanoindentation (Berkovich)



Cavity model: Effect of densification on pressure required for yield

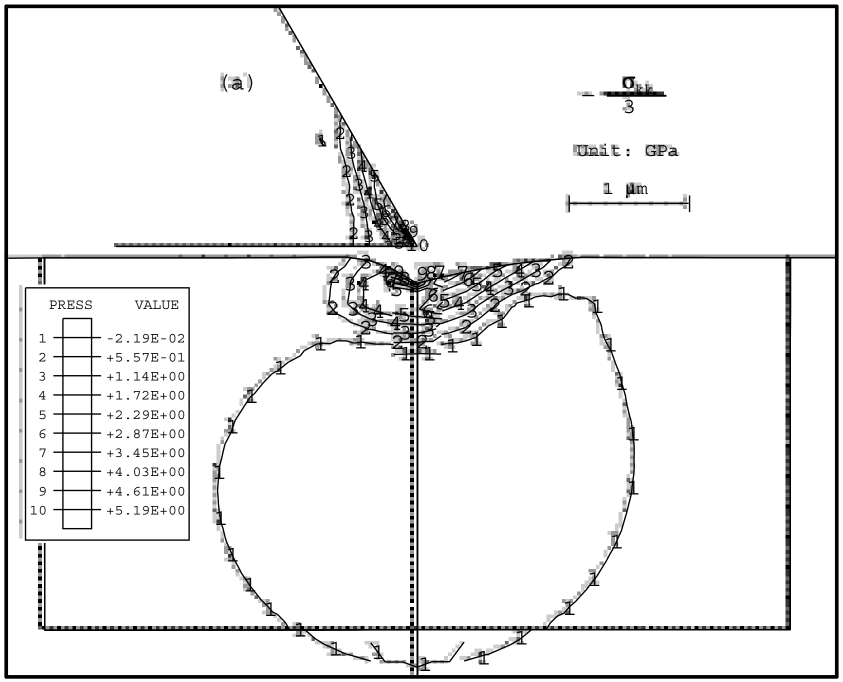


Cavity model: Densification effect on expansion

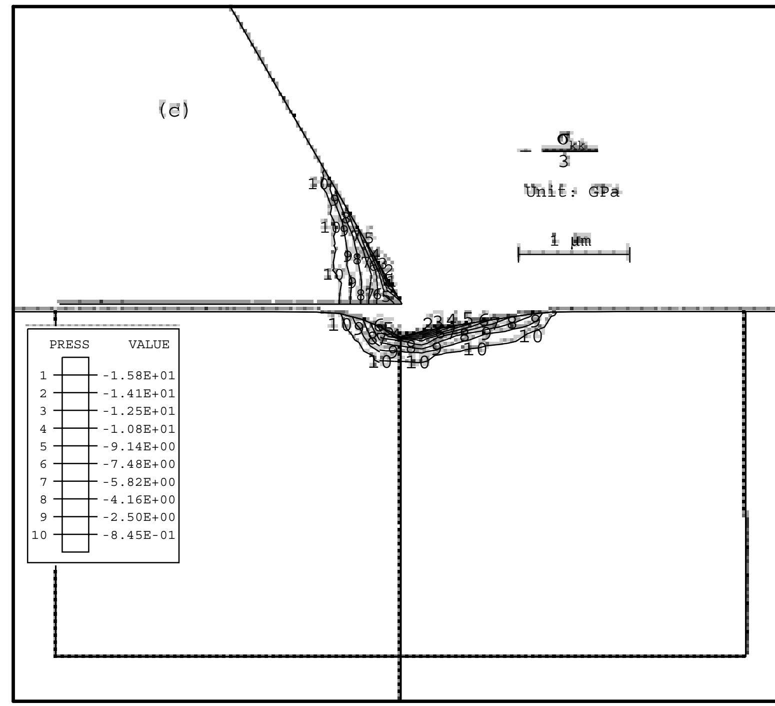


FEM analysis: Residual pressure under Berkovich

α= 0 (no densification)

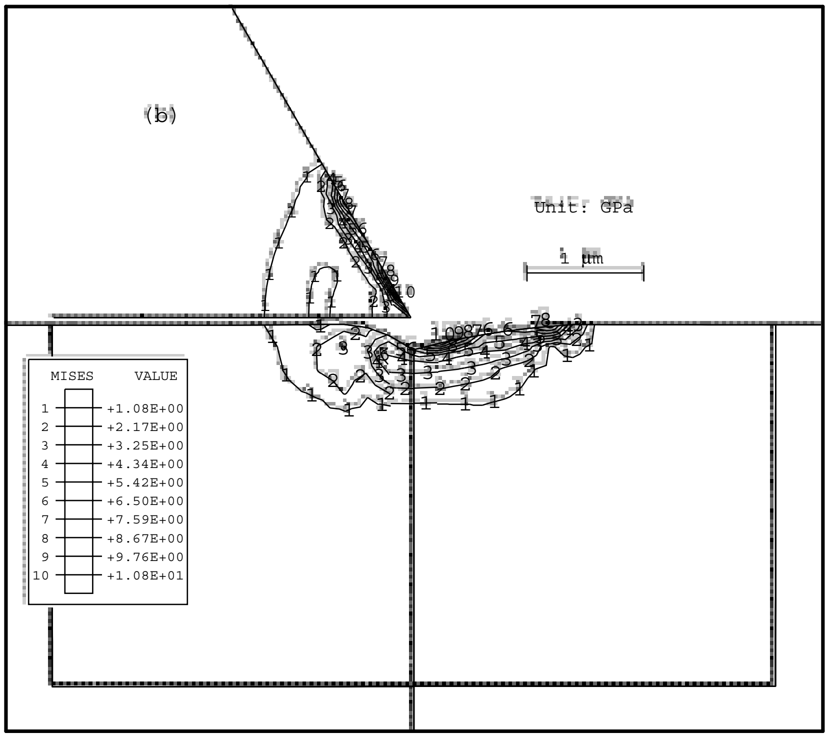


α = 0.6

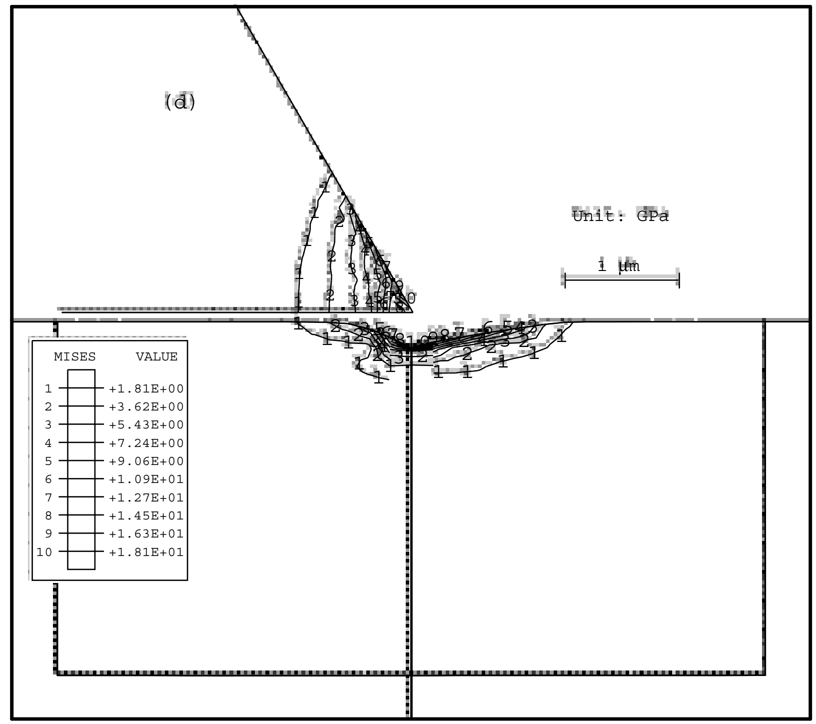


FEM analysis: Residual von-Mises stress

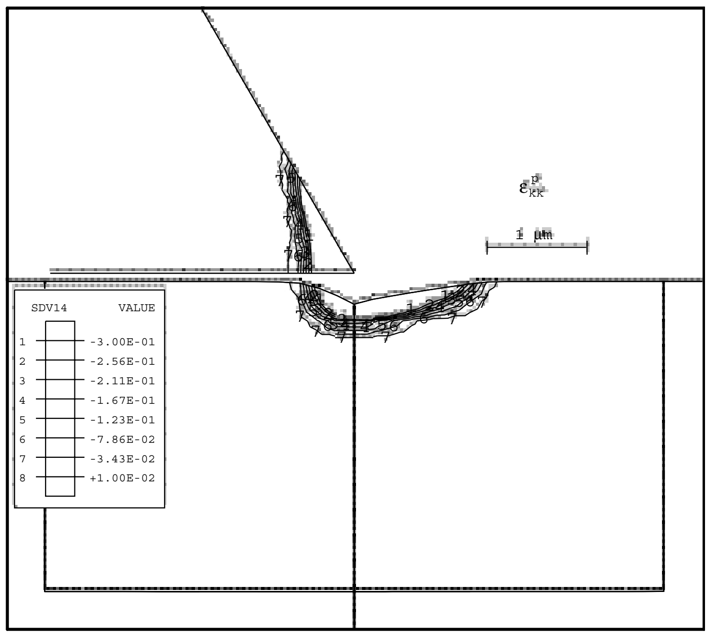
α = 0 (no densification)



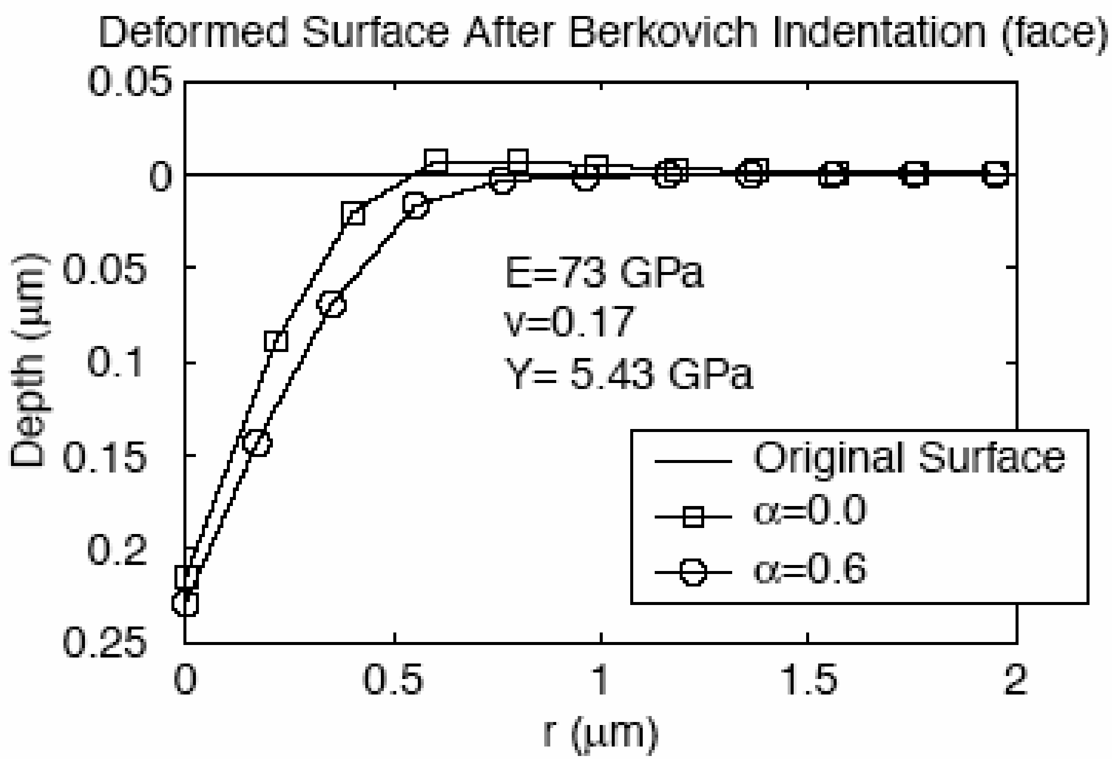
α= 0.6



FEM analysis: permanent densification for α = 0.6 Berkovich tip, F = 30 mN



FEM analysis: Indent surface topography



FEM analysis: Indent surface topography

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At P = Pmax (fully load)

First Pmax, then fully unload

QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.

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are needed to see this picture.

MD: EFFECTS OF LASE IRRADIATION

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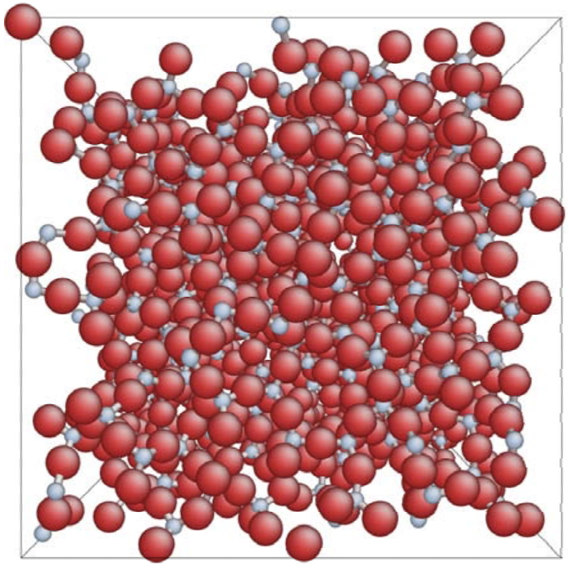
NVE: Constant energy & constant V

NVT: Constant volume and constant temp.

Nth: Constant stress and constant enthalpy

NtT: Constant stress and constant temp.

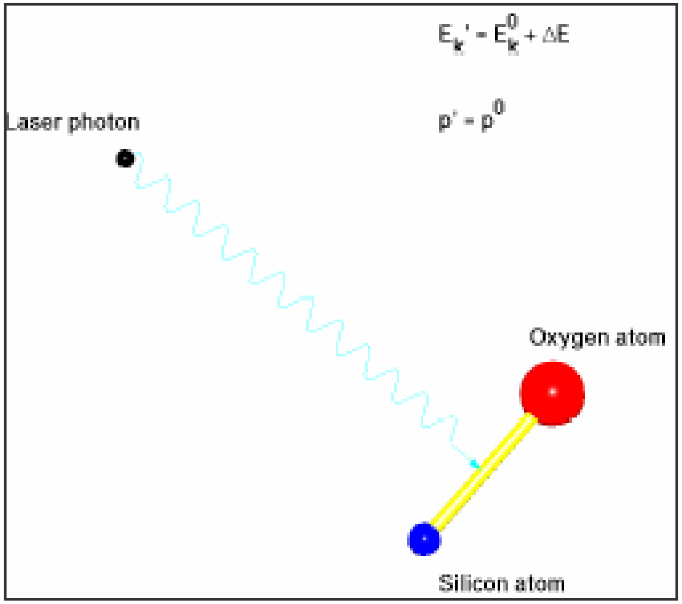


NUMERICAL MODEL FOR LASER INTERACTION

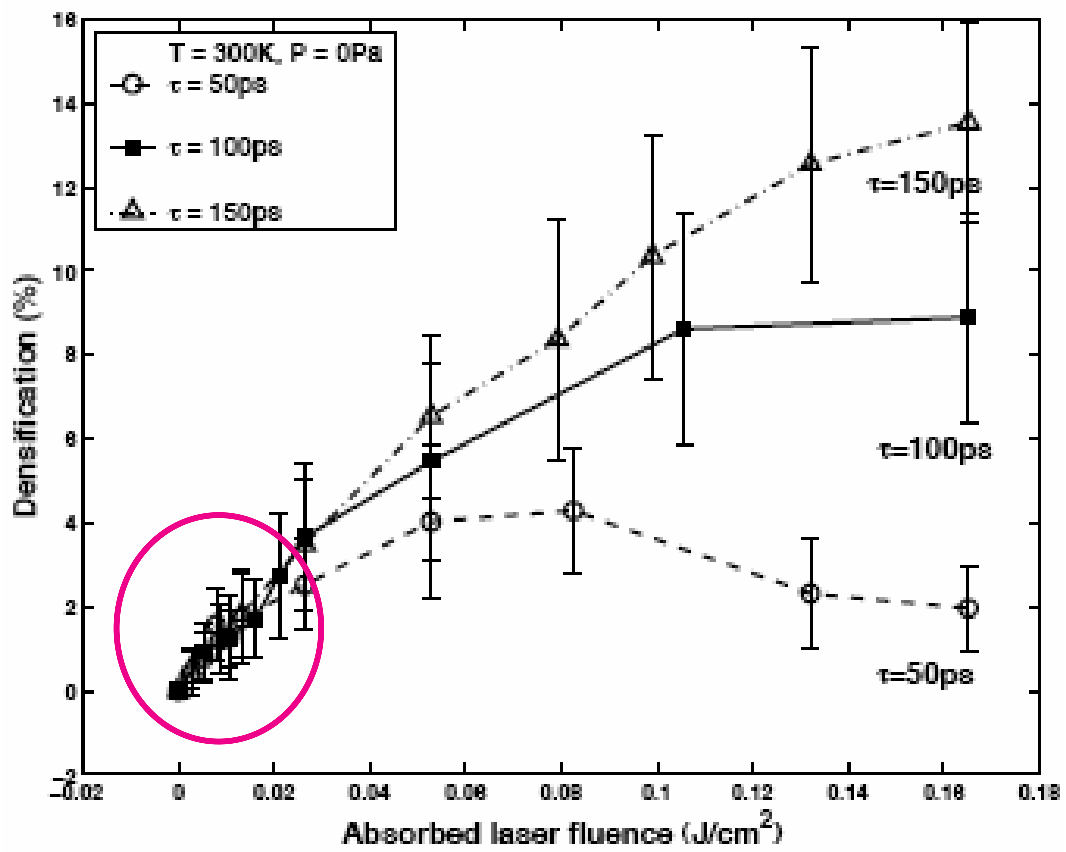
Potential energy for silica

(modified BKS potential: van Beest, 1955; Saika et al., 2000)

$$U(r_{ij}) = \underbrace{k_C \frac{q_i q_j}{r_{ij}}}_{\text{Coulomb}} + \underbrace{A_{ij} e^{-b_{ij} r_{ij}} - \frac{c_{ij}}{r_{ij}^6}}_{\text{Buckingham}} + \underbrace{4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{30} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]}_{\text{30–6 Lennard–Jones}}$$



MD LASER IRRADIATION: Effect of pulse duration & absorbed fluence @ T = 300 K, p = 0 GPa



MD LASER IRRADIATION: Effect of pulse duration @ T = 300 K, p = 0 GPa

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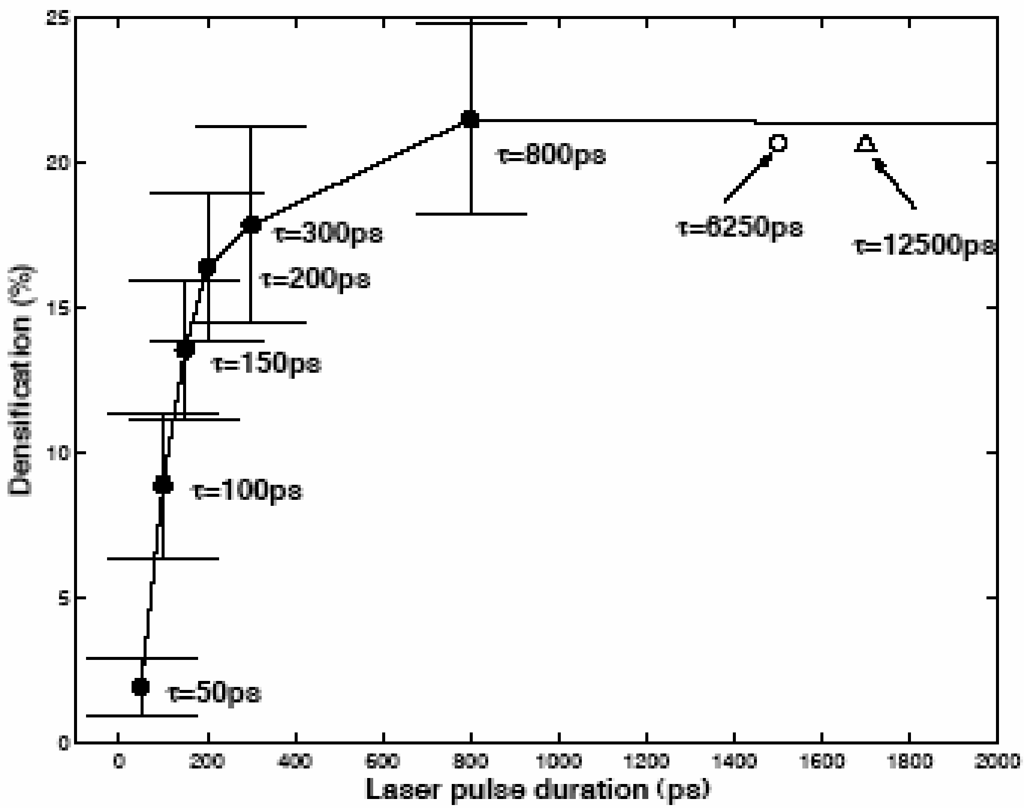
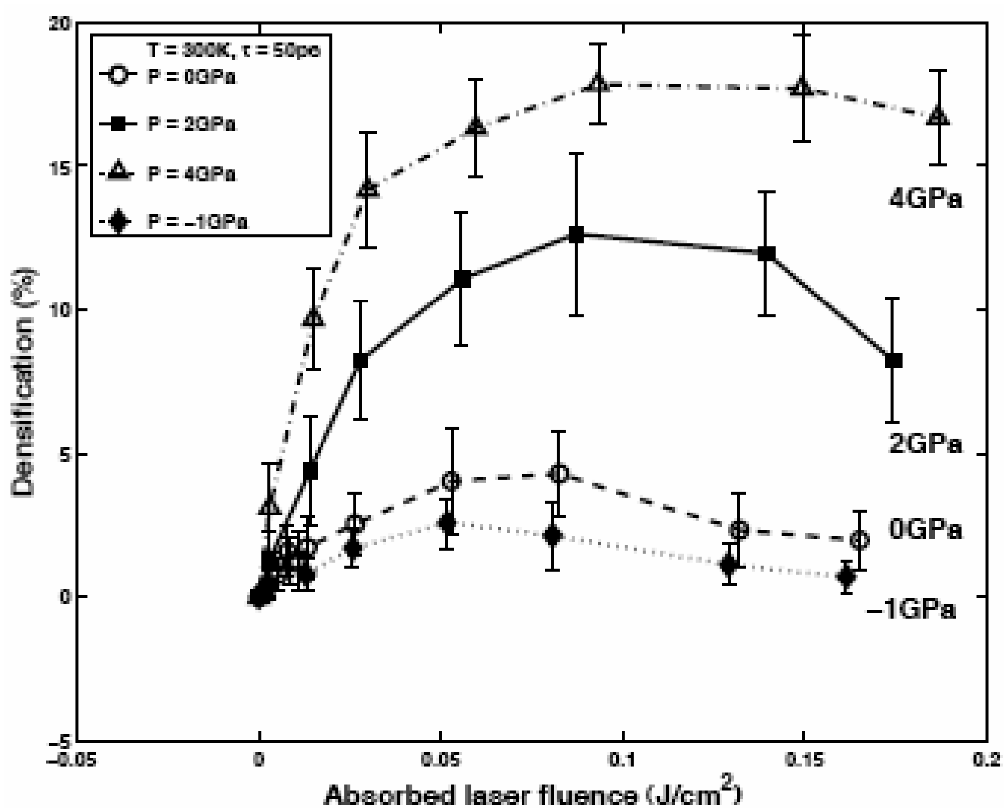
Absorbed fluence = 0.165 J/cm^2

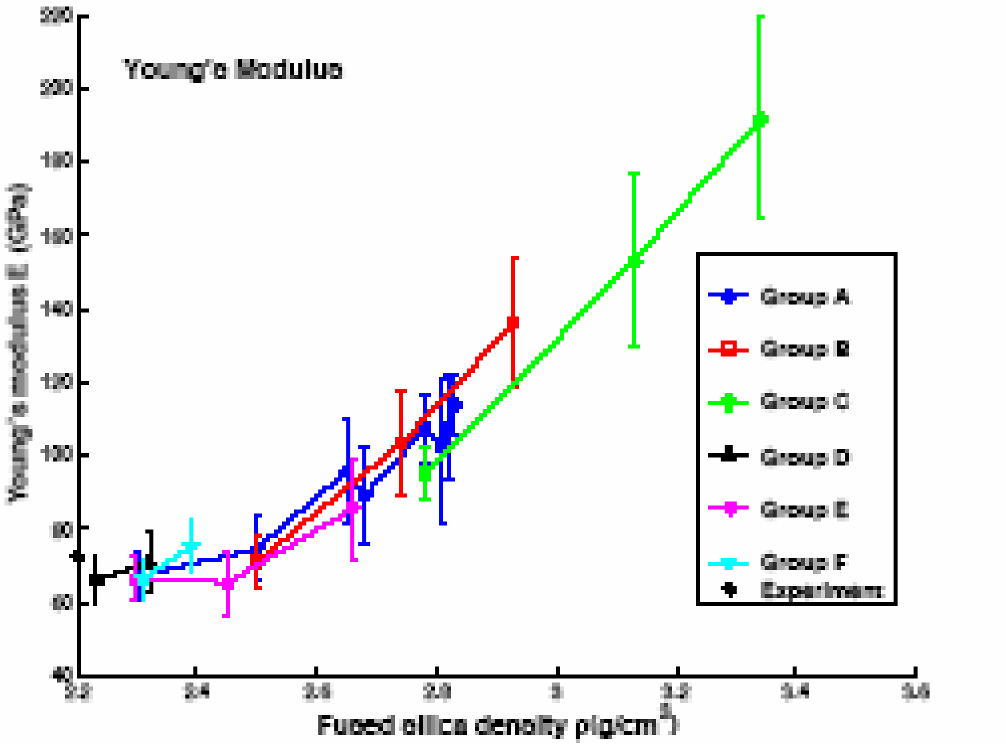


MD LASER IRRADIATION: Effect of pressure @T = 300 K

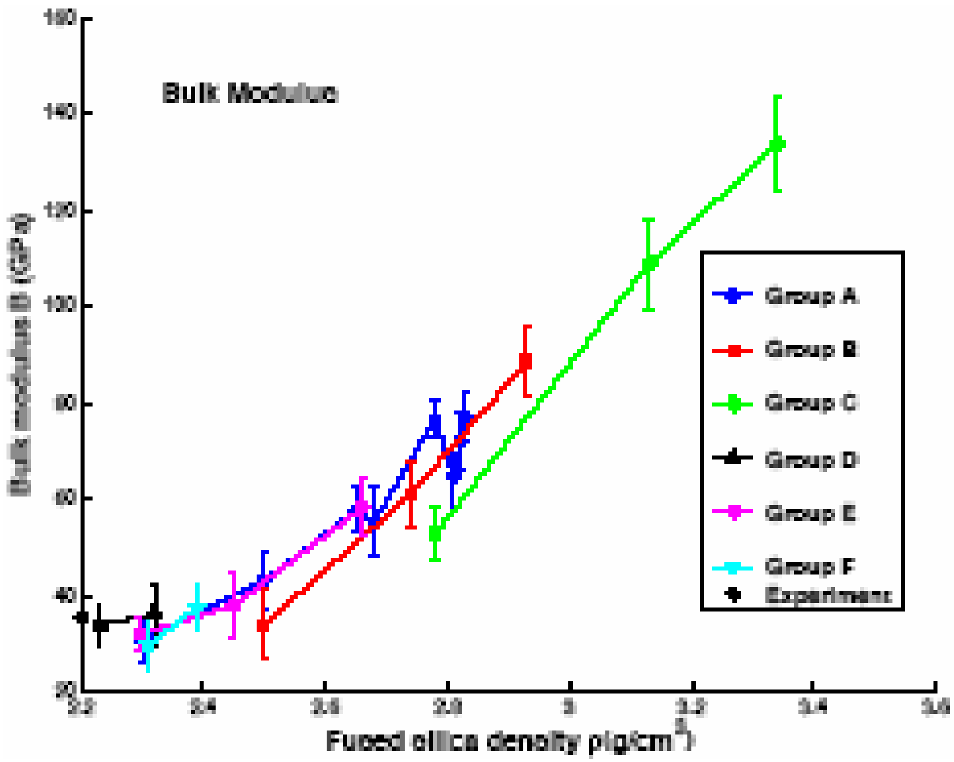
Higher pressure produces higher densification



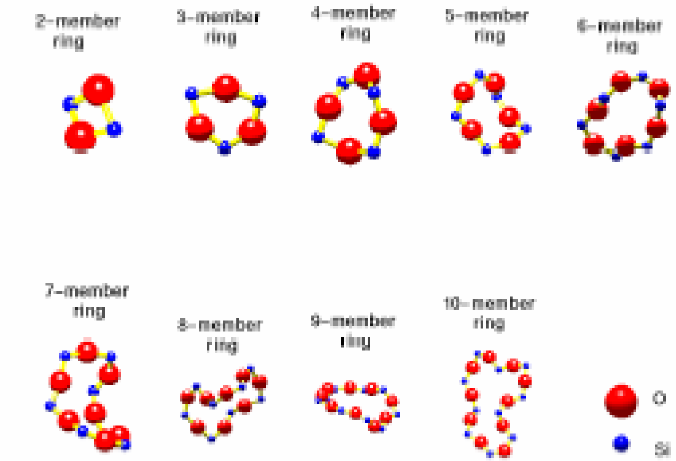
MD simulations: Effect of radiation on Young's modulus

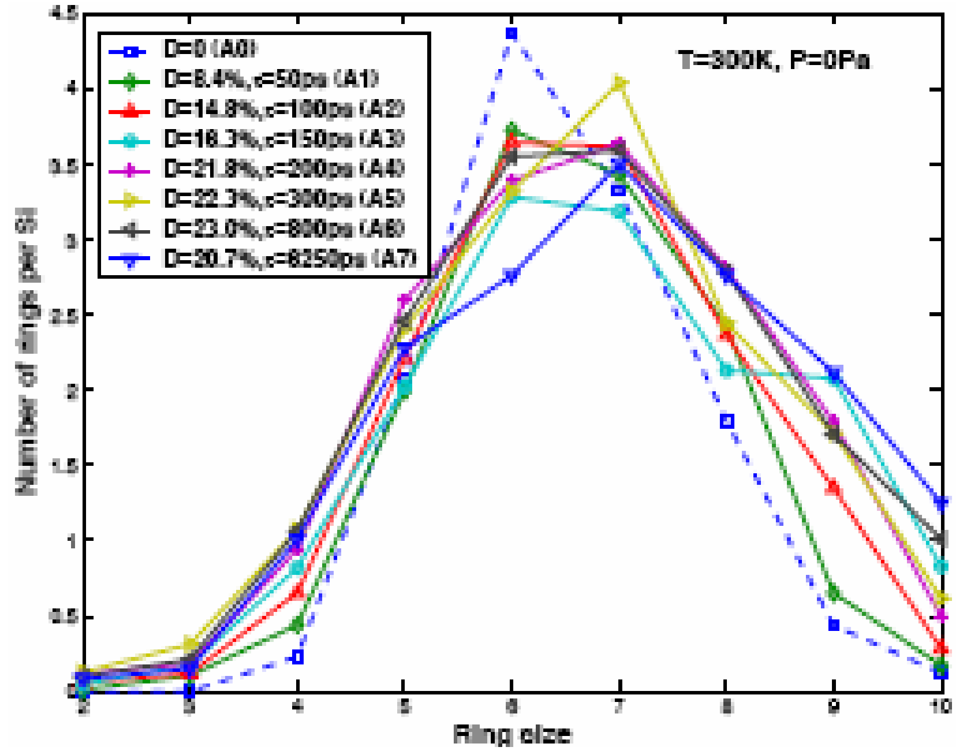


MD simulations: Effect of radiation on bulk modulus B



MD simulations: Effect of radiation on glass structure





CONCLUSIONS

CONSTITUTIVE LAW:

Yield function, flow potential, hardening

INDENTATION:

Load-displacement curves, residual stresses, topography,

Effect of densification on hardening

Grinding, Polishing

MD SIMULATIONS: Laser-induced densification

Effects of pulse duration, fluence, temperature, pressure on

Densification, elastic moduli