



DENSIFICATION OF FUSED SILICA BY STRESS OR LASER IRRADIATION

John C. Lambropoulos

**Dept. Mechanical Eng'ng, Materials Science Program,
& Laboratory for Laser Energetics**

University of Rochester, Rochester, NY 14627

**Contributions: Kang-Hua Chen, Lianjqing Zheng,
Joe Randi, Kai Xin, Ed Fess, Steve Jacobs & Ansgar Schmid**

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**

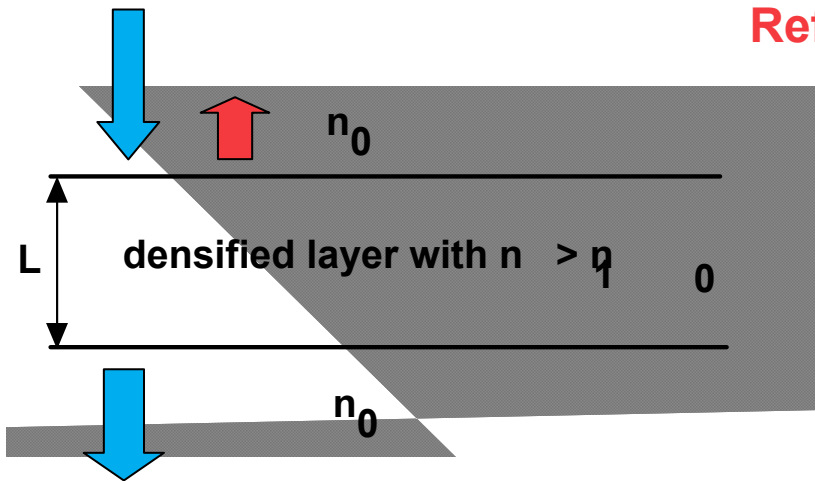
- **MD SIMULATIONS: laser-induced densification**
- **Fluence, pulse duration, elastic moduli**

POLISHING OF FUSED SILICA & IMPLICATIONS

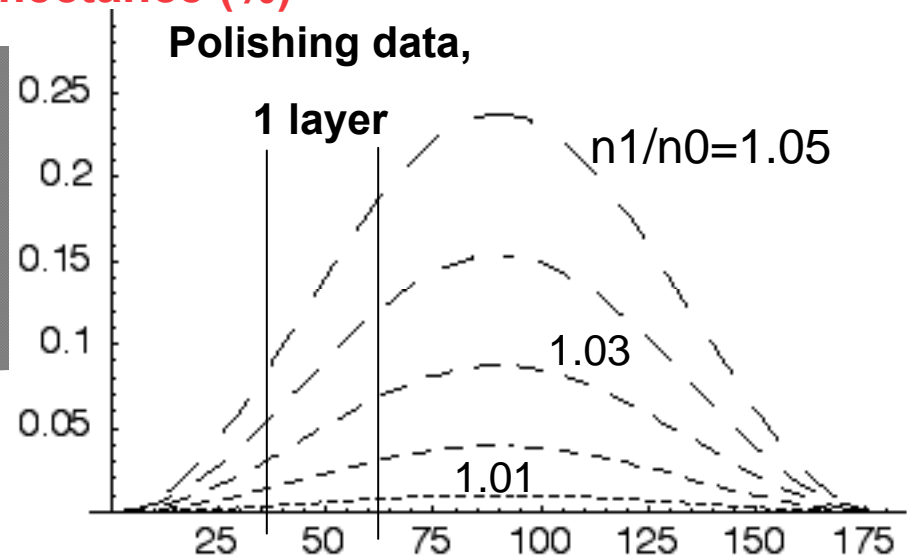
(Yokota et al., 1969; Malin & Vedam, 1977)

Ellipsometric measurement of index of refraction

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



Reflectance (%)



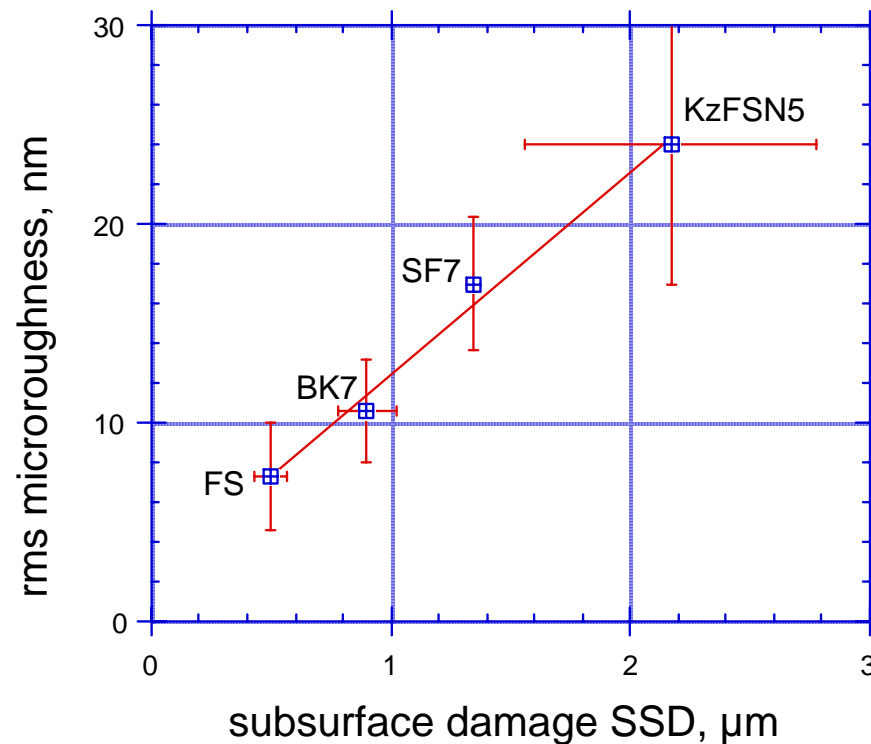
Phase $\delta = 360 n_1 L/\lambda$ (degrees)

DETERMINISTIC MICROGRINDING(Rochester, 1993-98)

2-4 μm bound diamond abrasive tool

Infeed rate $\sim 6 \mu\text{m}/\text{min}$

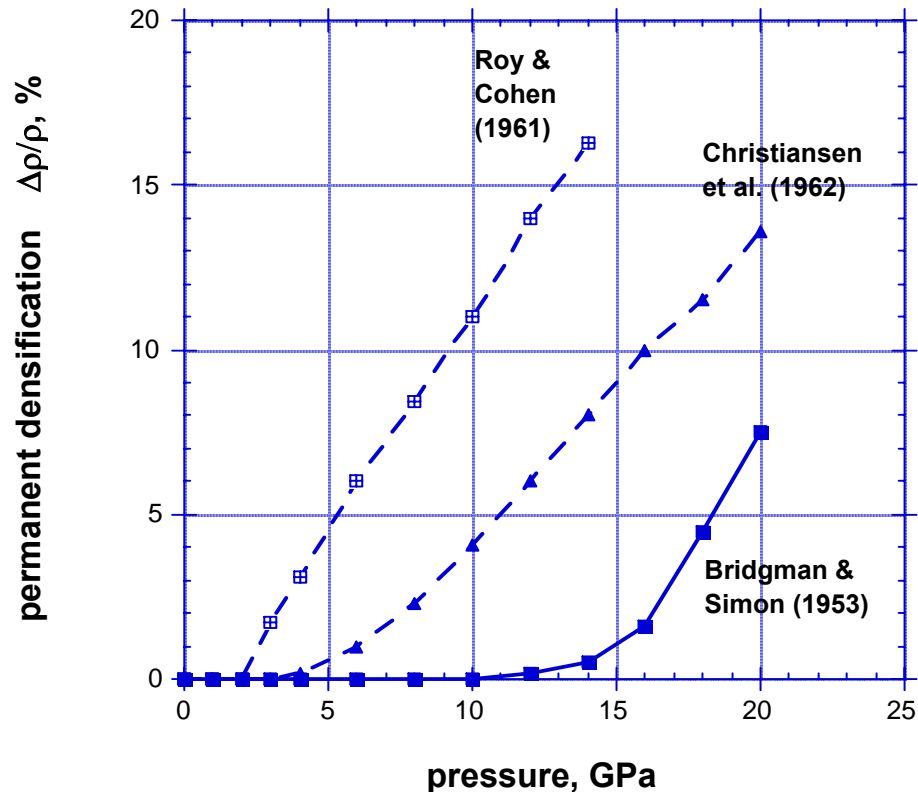
FS produces superior finish, minimal subsurface damage



PERMANENT DENSIFICATION

Effects of pressure (and shear)

Permanent densification of fused silica @ 25 °C °C

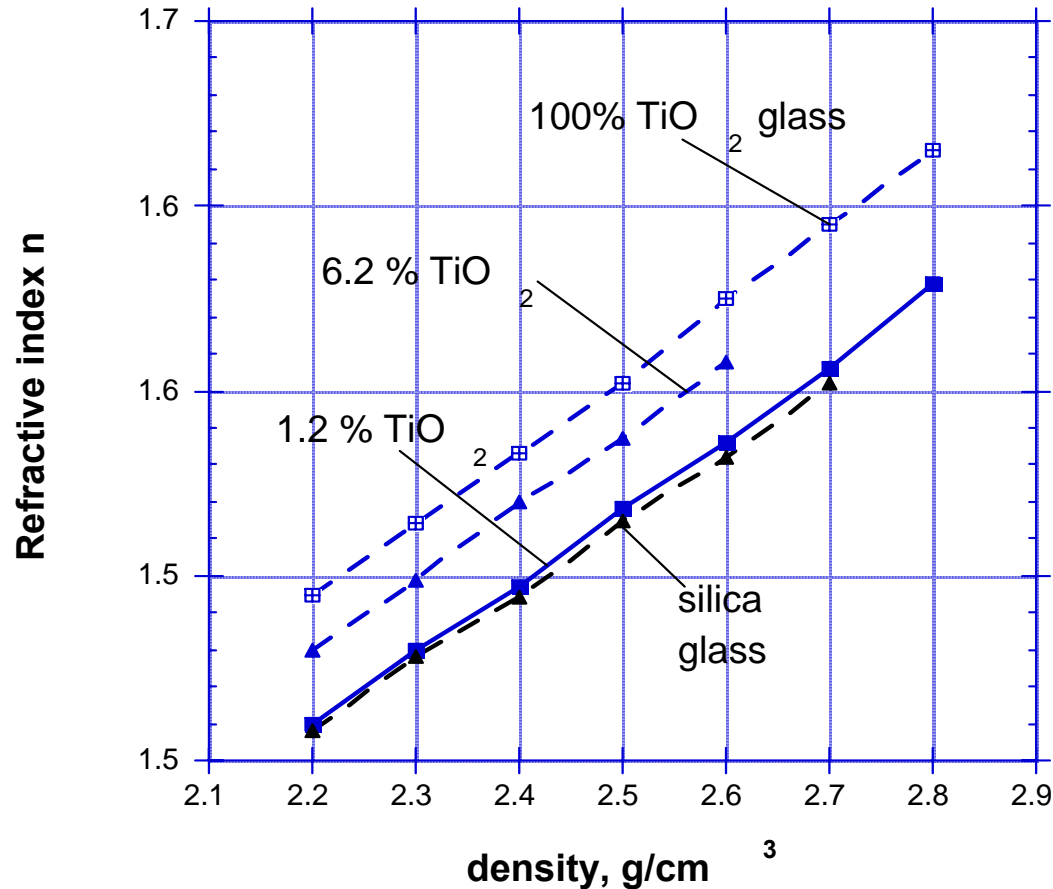


Pressure transmitting medium in high pressure cell:

Al₂O₃ (high shear) vs AgCl (low shear)

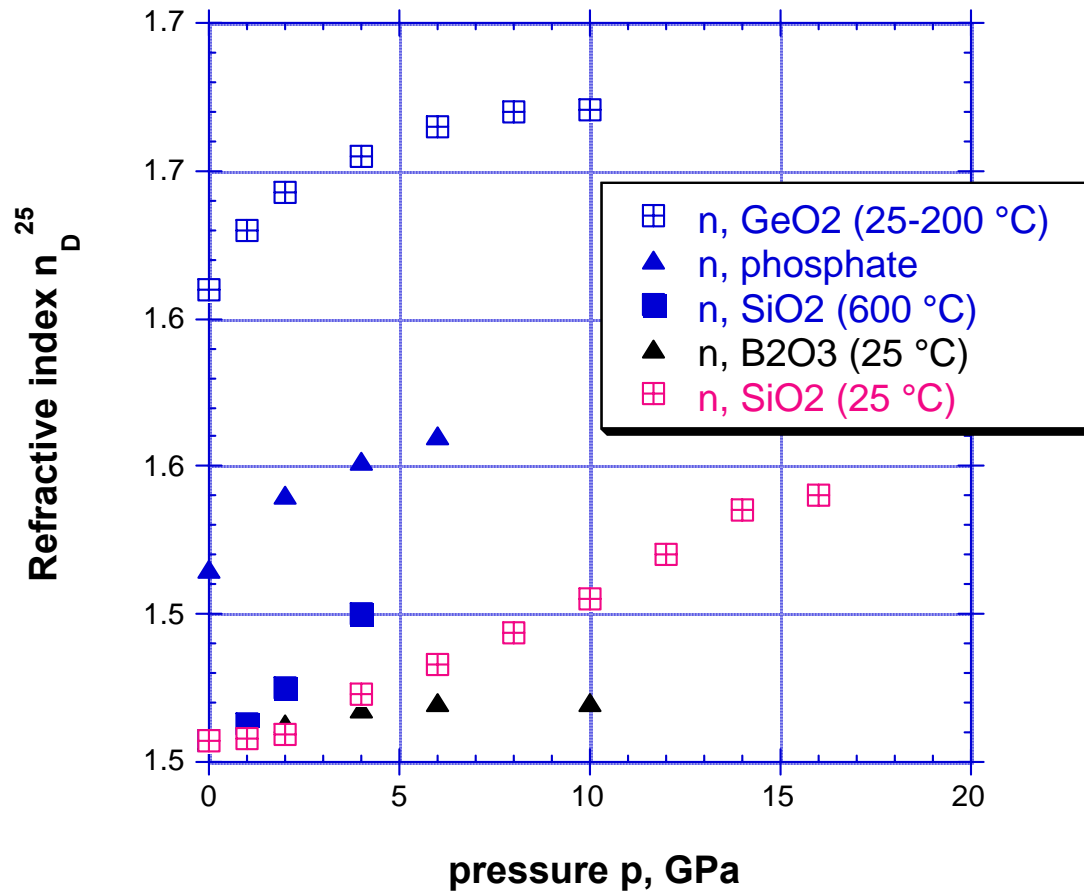
EFFECT OF DENSIFICATION ON n: $\Delta n/\Delta\rho \sim 0.025 \text{ 1/(g/cc)}$

n vs. ρ in densified glasses
(Arndt, 1983)



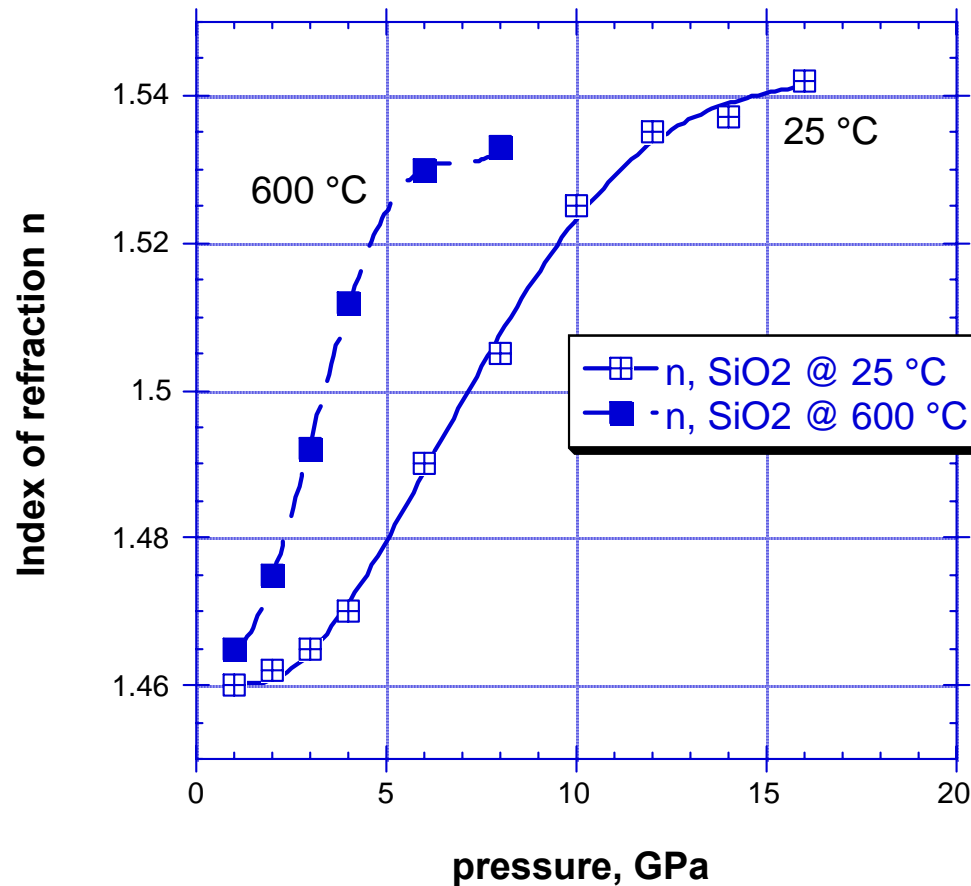
Different glasses densify: n vs pressure

n vs densification pressure
(Cohen & Roy, 1961)



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

Effect of pressure & temperature on densification

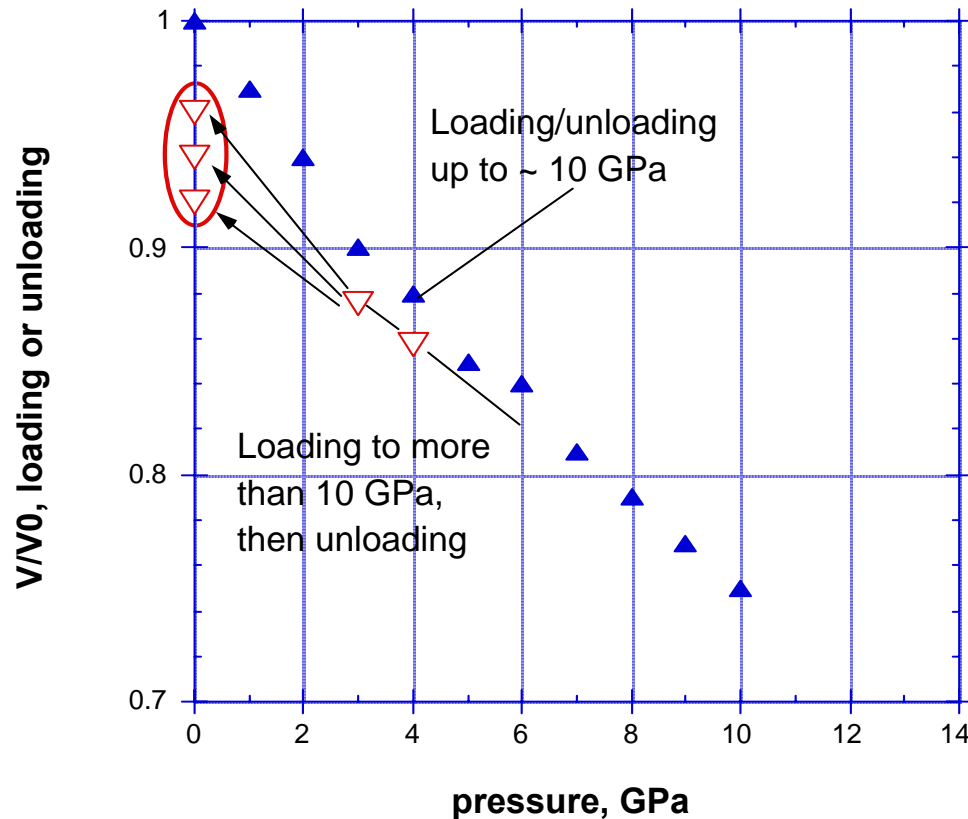


Volume strain vs pressure in fused SiO₂ (Meade & Jeanloz, 1987)

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)



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:

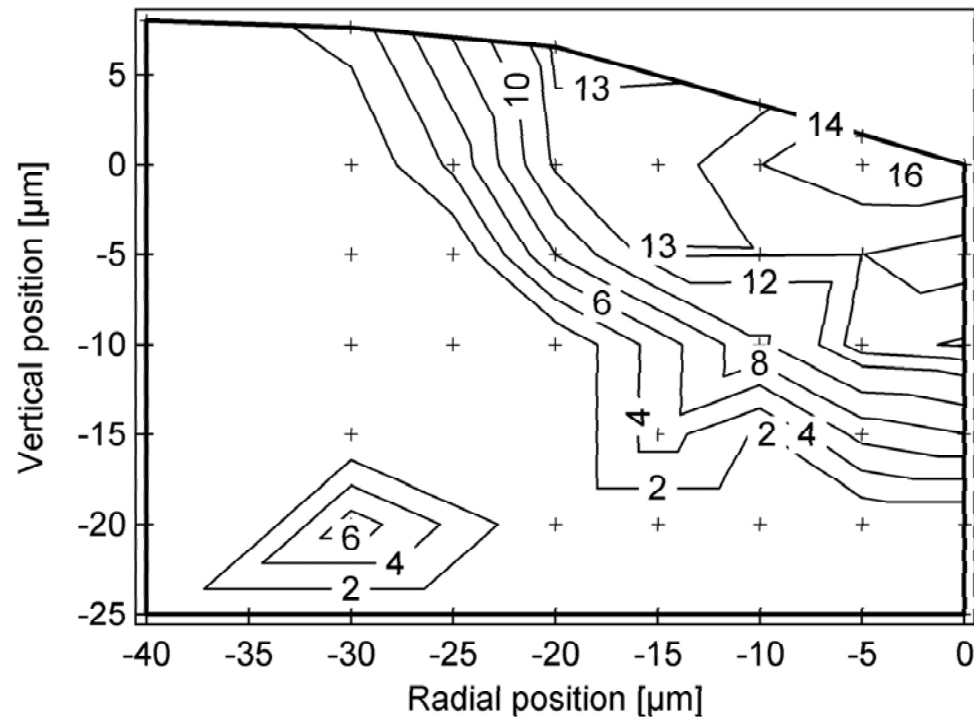
Absence of shear flow lines,

Absence of pile up around indent edge

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

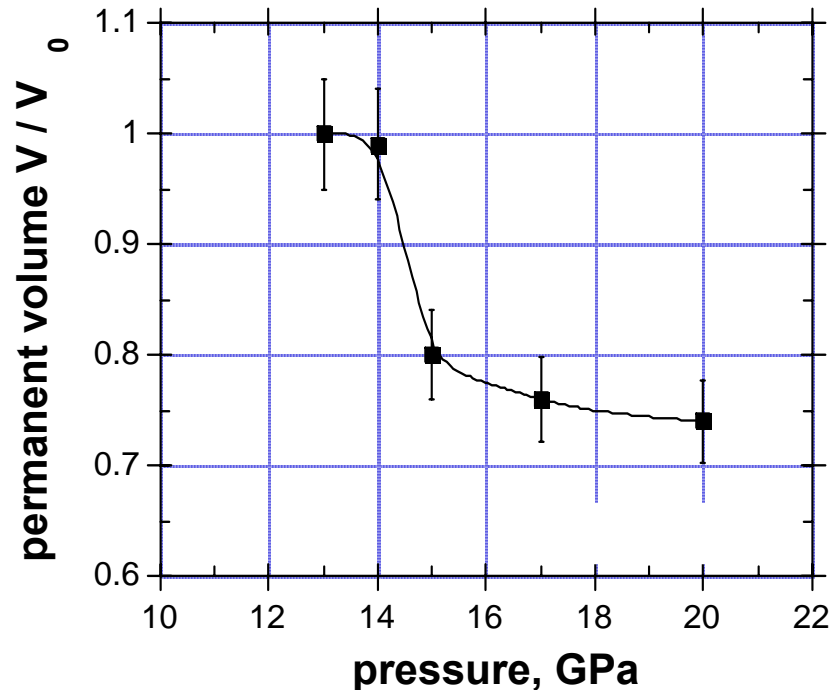
Iso-densification lines for $\Delta\rho/\rho_0$ (%) under indent :

Densification from 2-16 %



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

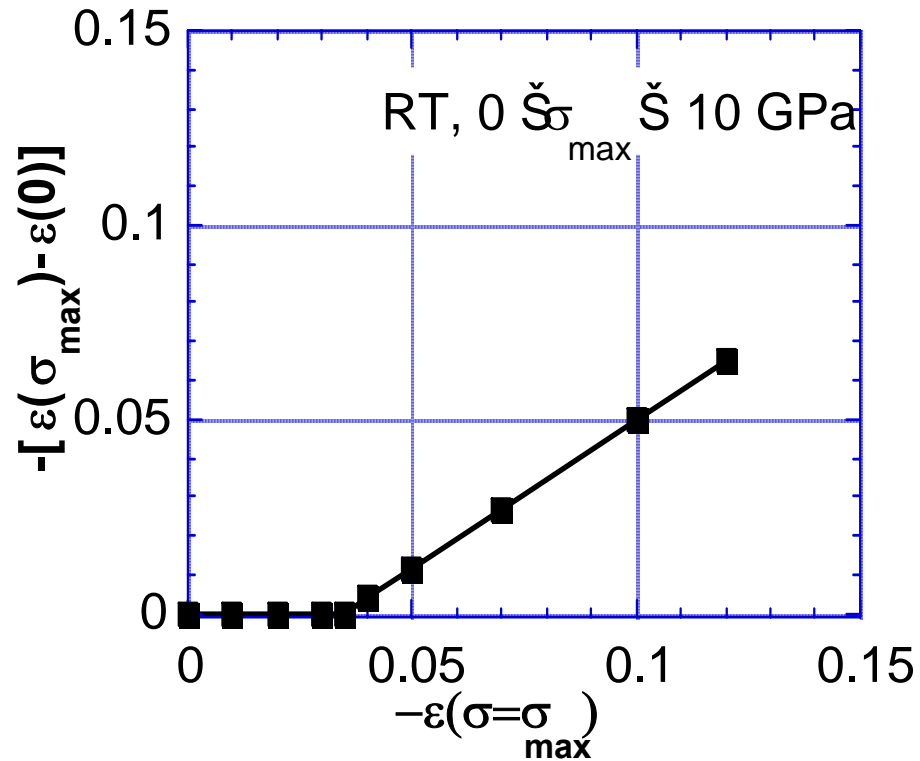
Si coordination number increases from 4 to ~ 6
as permanent volume V decreases from V_0 to $\sim 0.75 V_0$



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

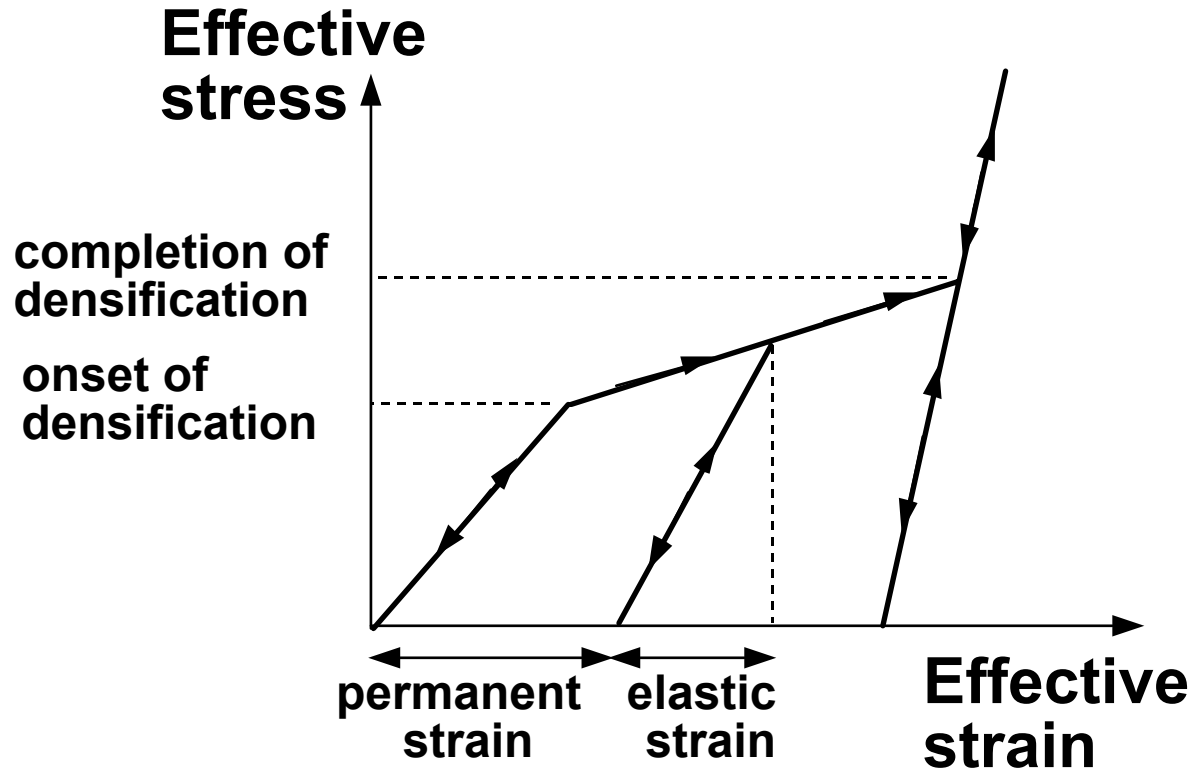
Plastic (i.e. permanent) strain vs. total strain (i.e. max load)

“Permanent strain”



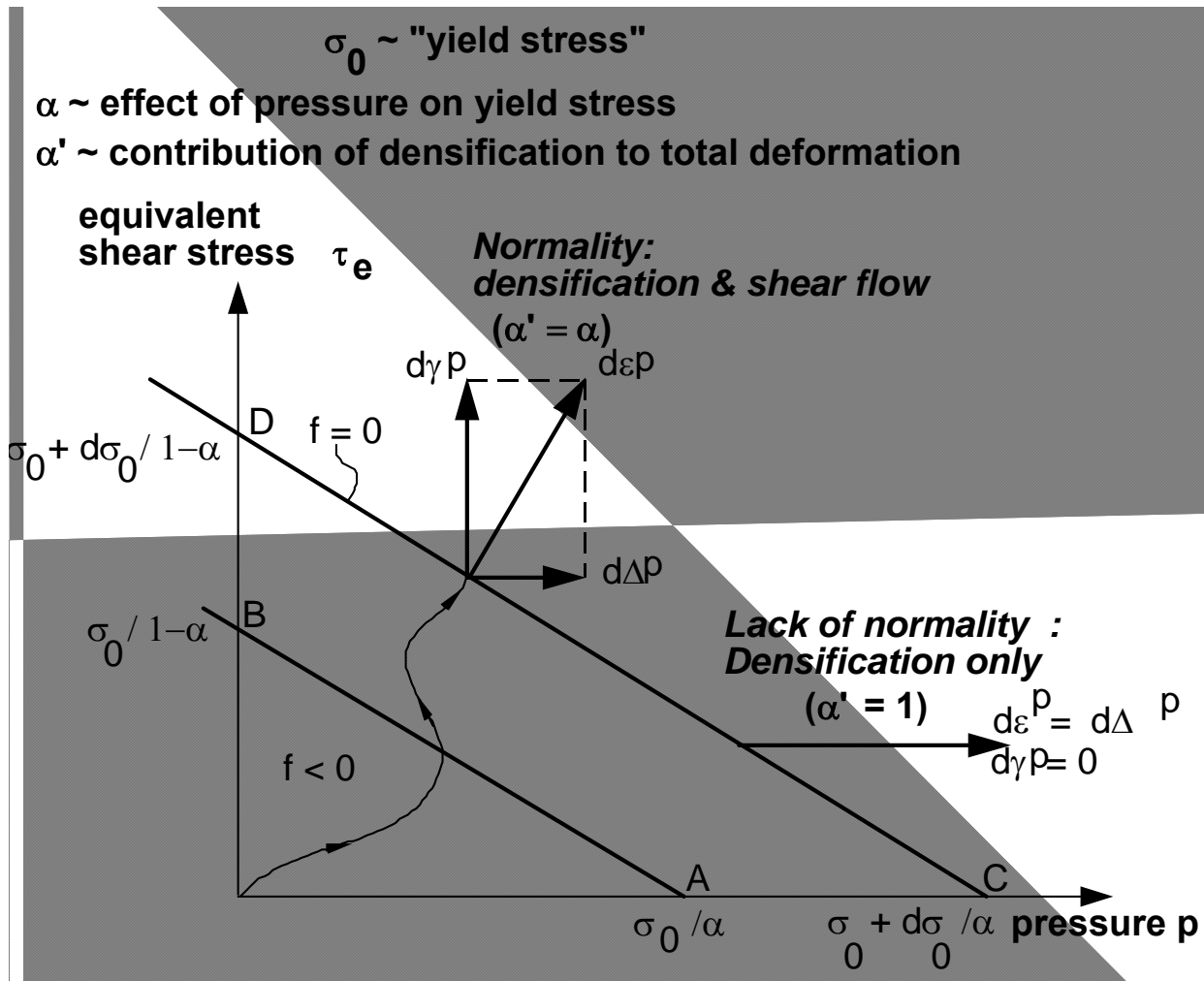
“max load”

CONSTITUTIVE LAW: Stress-strain curve



CONSTITUTIVE LAW: FLOW RULE & HARDENING

hardening modulus $h = 14 - 32 \text{ GPa}$





DENSIFICATION OF FUSED SILICA BY STRESS OR LASER IRRADIATION

Part 2

John C. Lambropoulos

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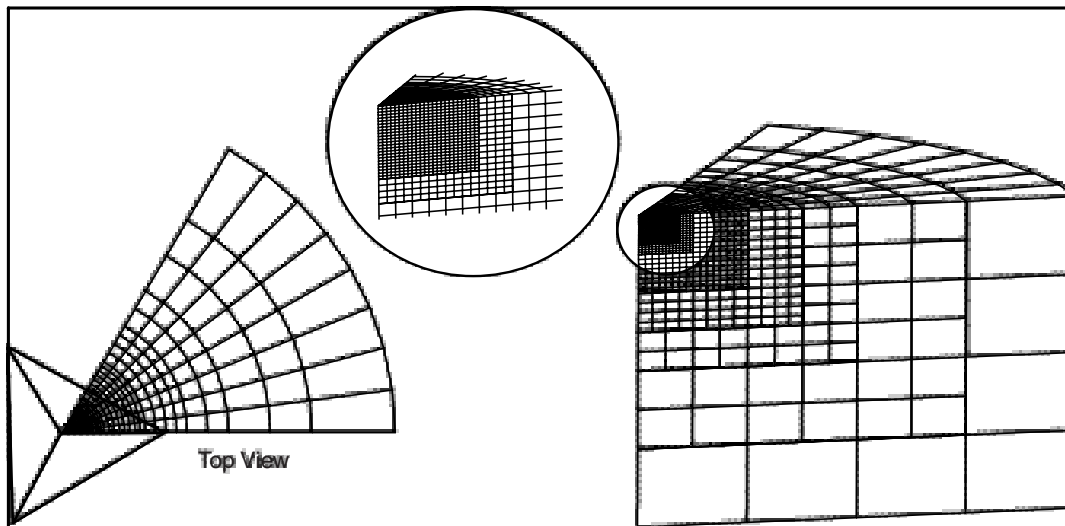
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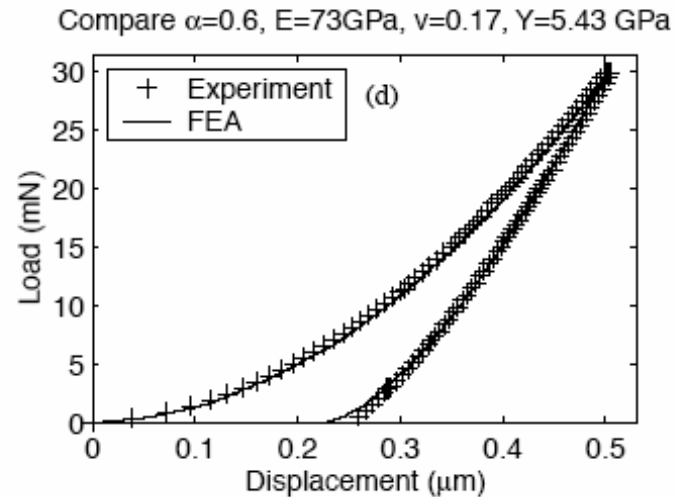
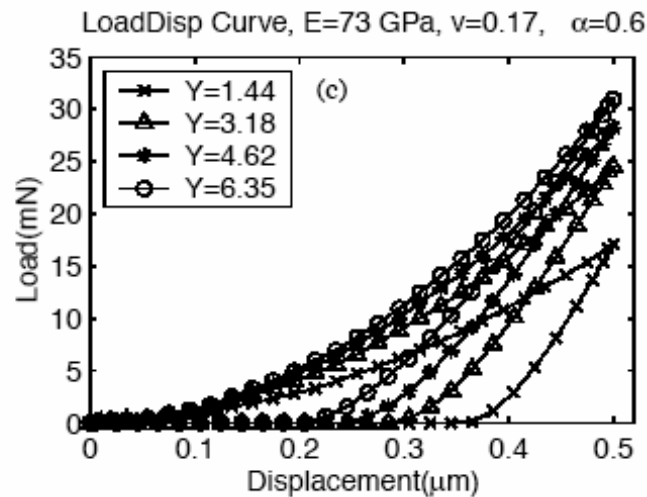
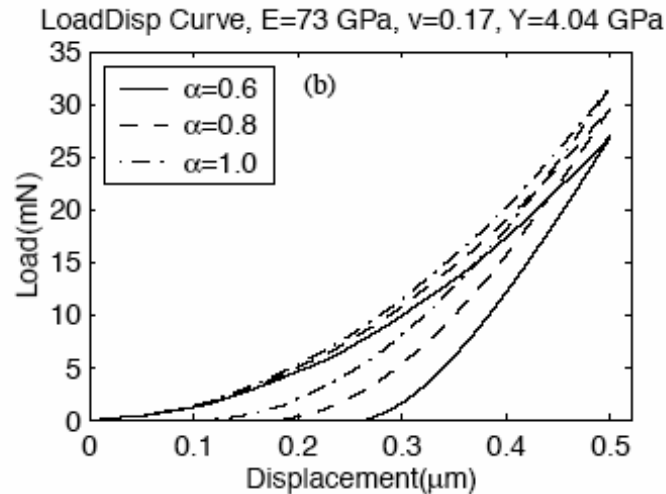
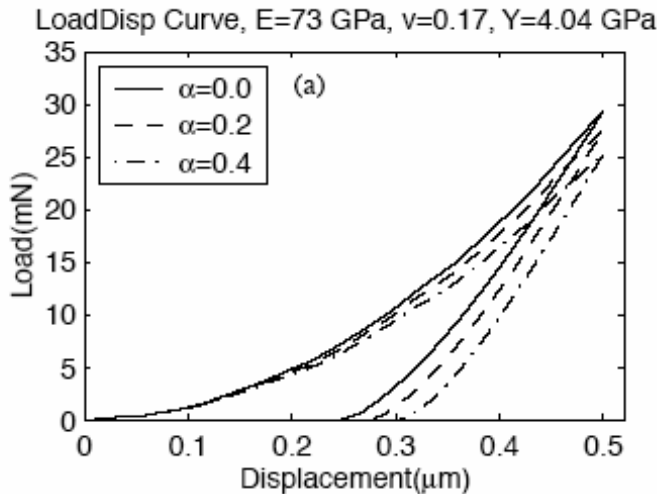
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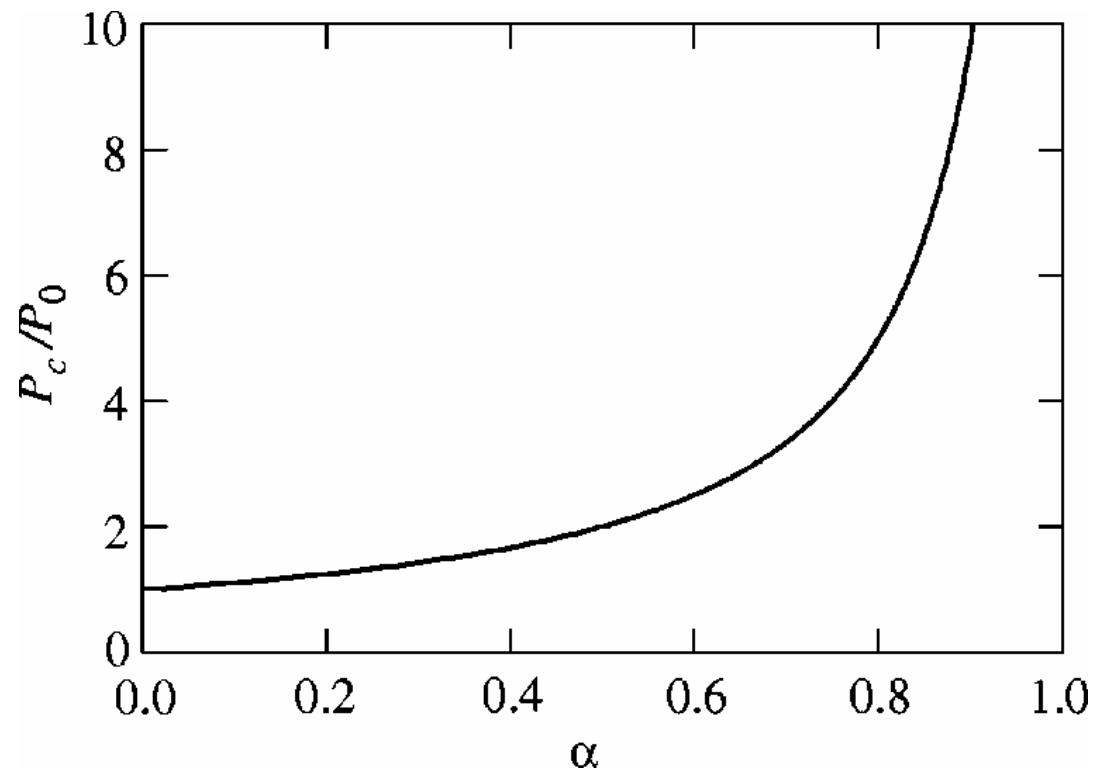
FEM analysis: 3D, Berkovich tip



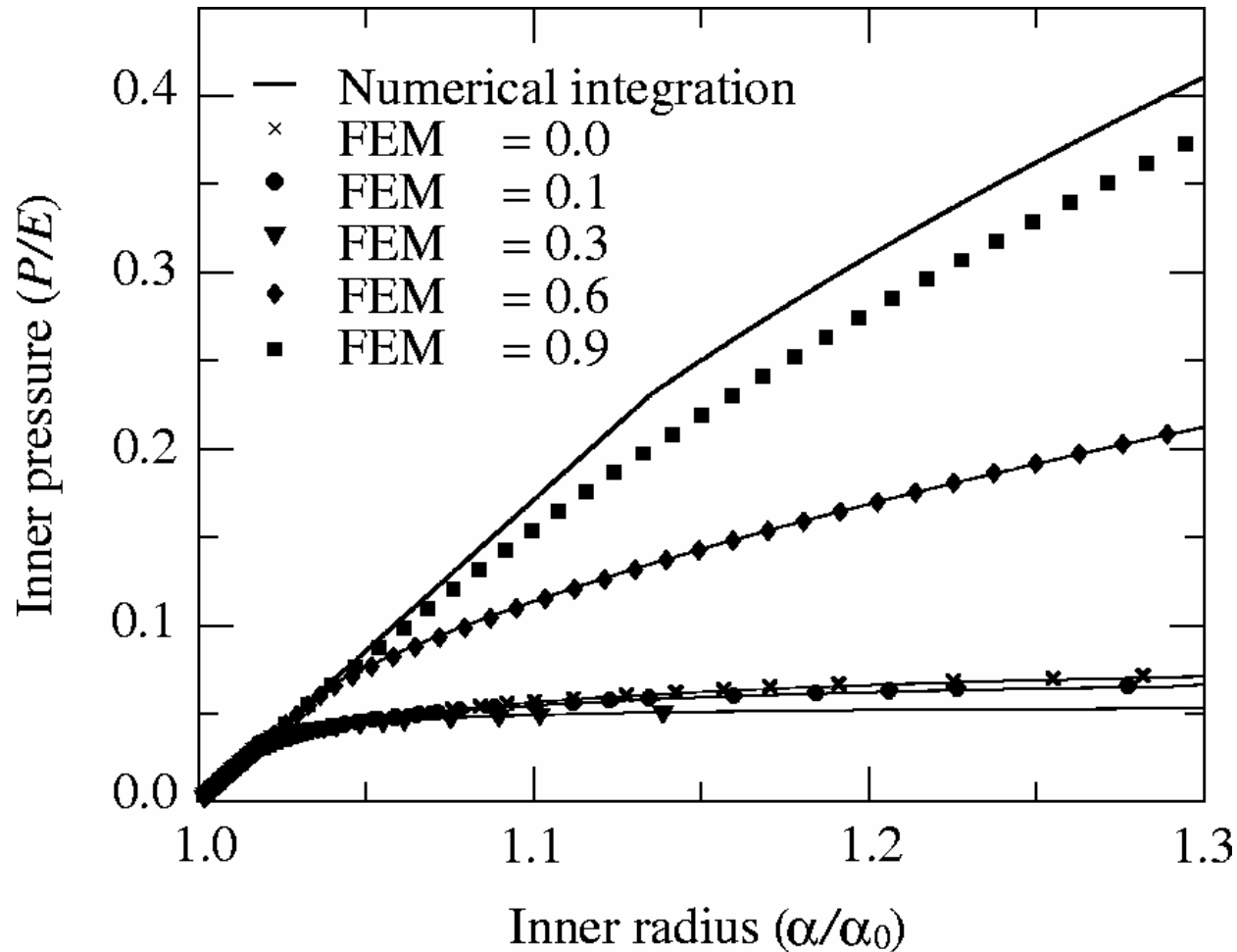
FEM analysis: Effect of densification parameter α & comparison with nanoindentation (Berkovich)



Cavity model: Effect of densification on pressure required for yield

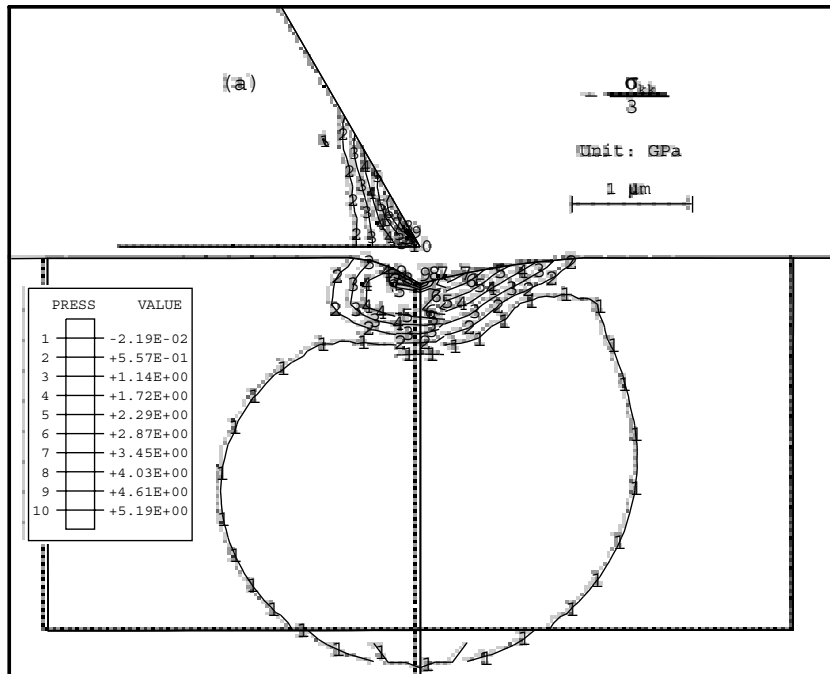


Cavity model: Densification effect on expansion

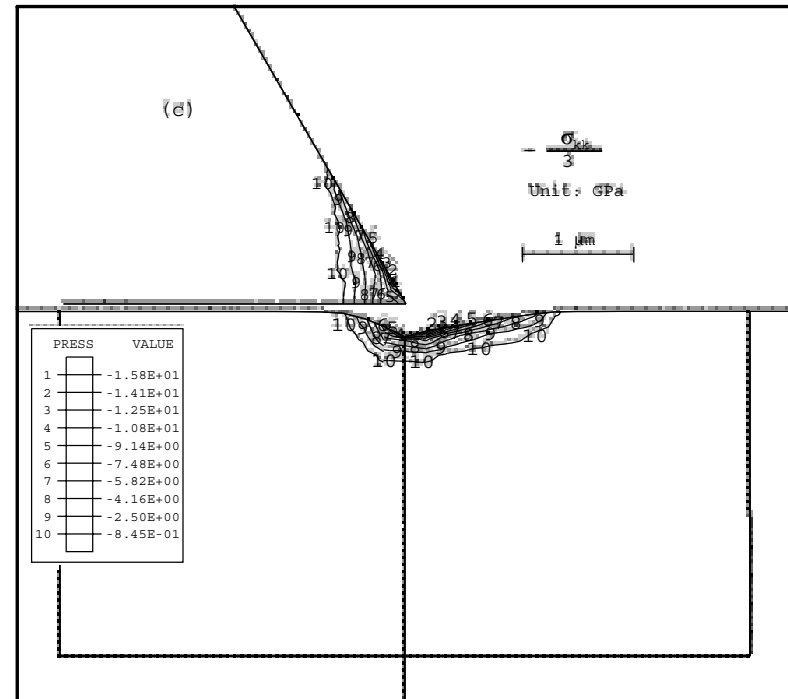


FEM analysis: Residual pressure under Berkovich

$\alpha = 0$ (no densification)



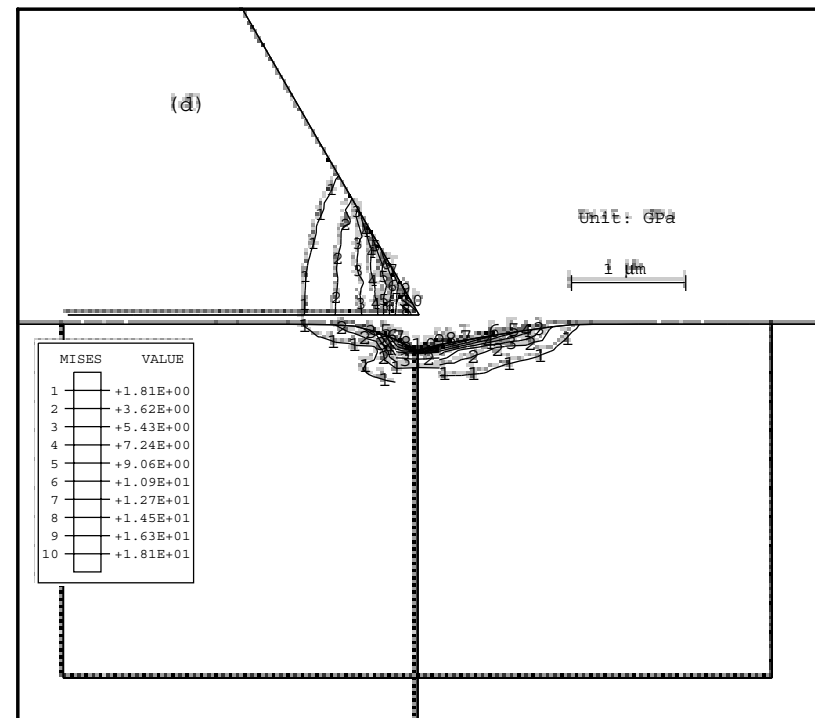
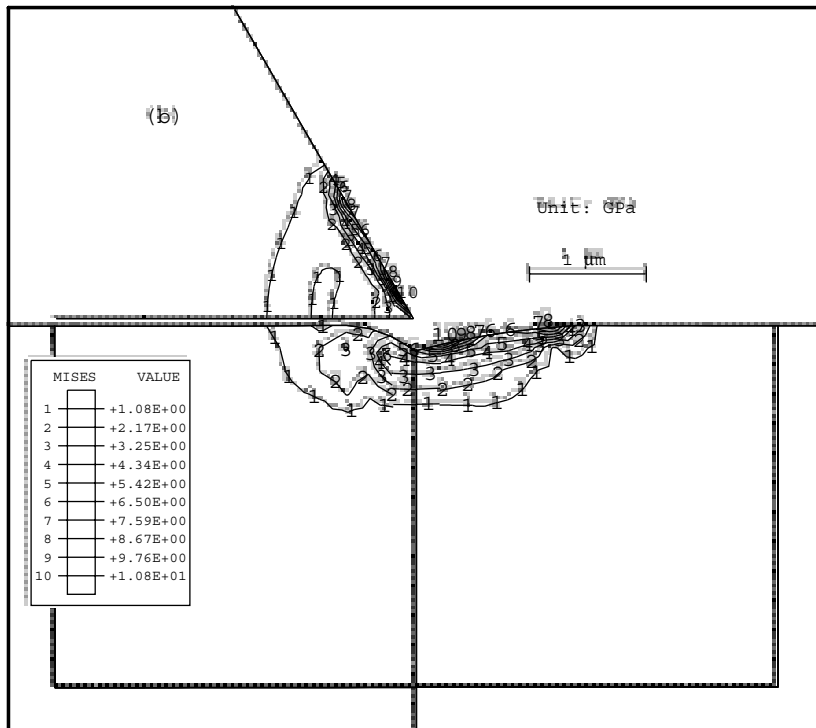
$\alpha = 0.6$



FEM analysis: Residual von-Mises stress

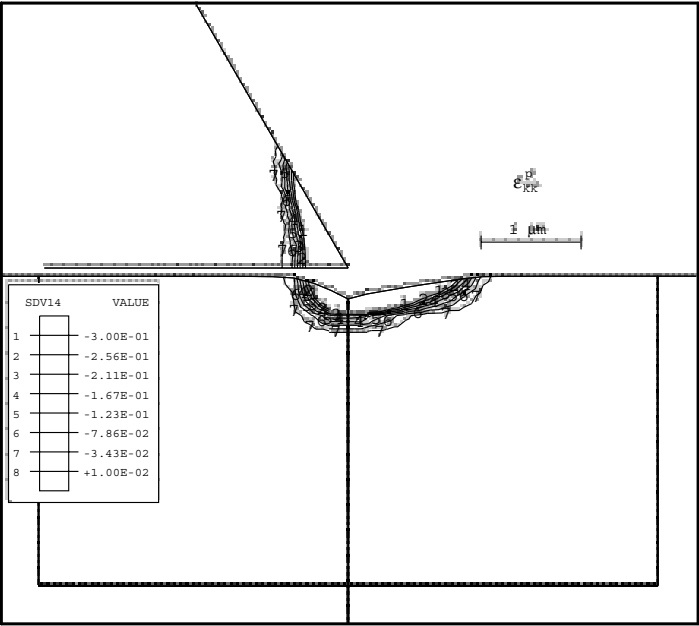
$\alpha = 0$ (no densification)

$\alpha = 0.6$

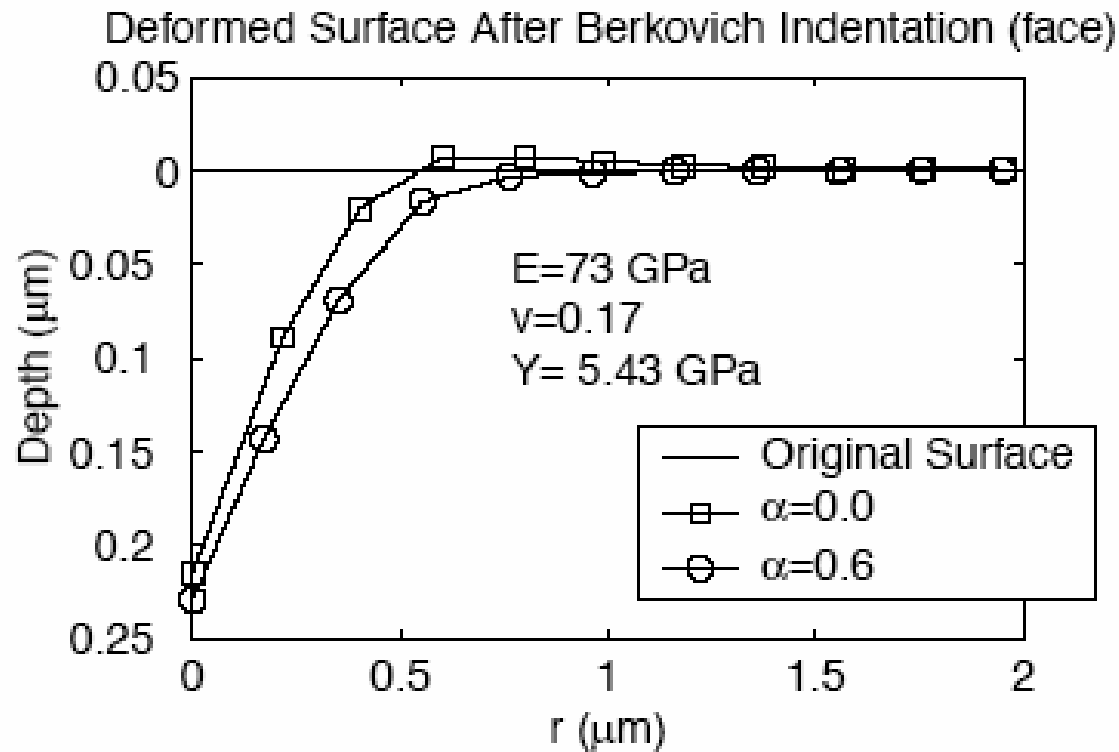


FEM analysis: permanent densification for $\alpha = 0.6$

Berkovich tip, $F = 30 \text{ mN}$



FEM analysis: Indent surface topography



FEM analysis: Indent surface topography



At $P = P_{max}$ (fully load)

First P_{max} , then fully unload

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

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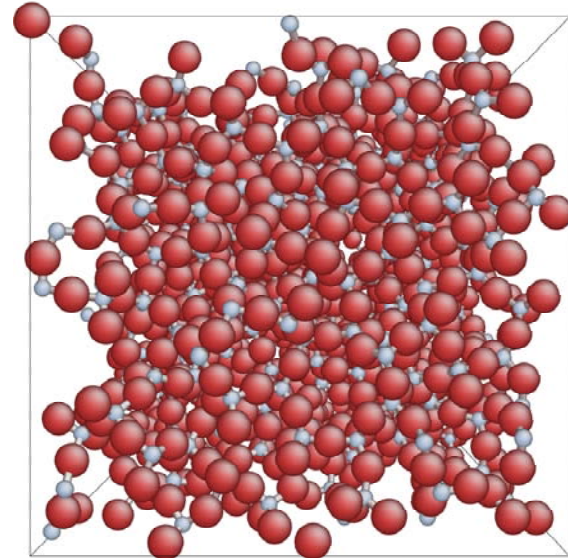
MD: EFFECTS OF LASE IRRADIATION

NVE: Constant energy & constant V

NVT: Constant volume and constant temp.

Nth: Constant stress and constant enthalpy

NtT: Constant stress and constant temp.

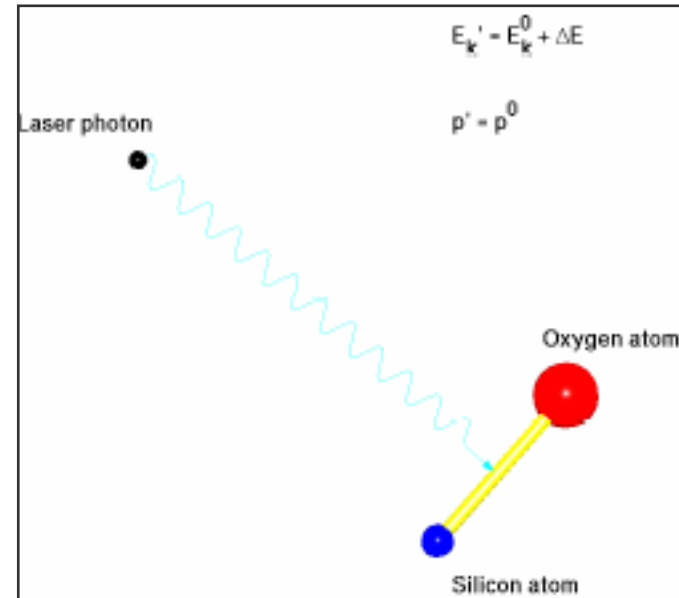


NUMERICAL MODEL FOR LASER INTERACTION

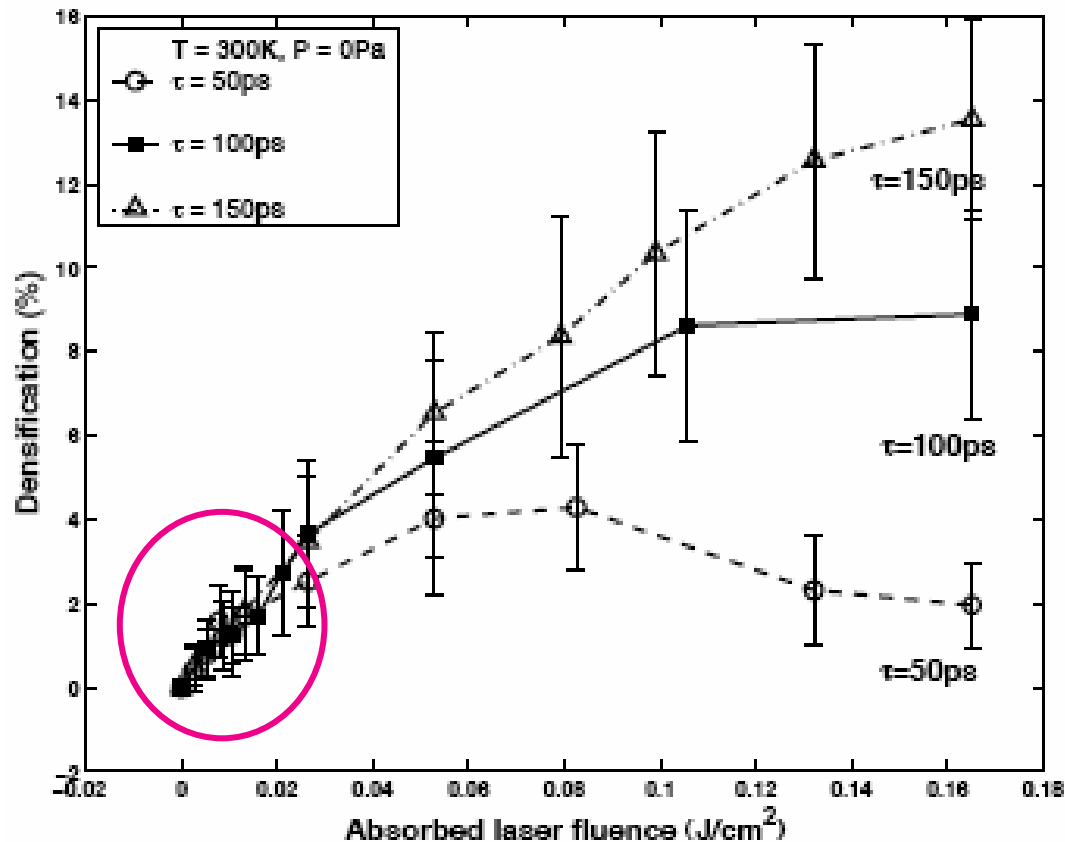
Potential energy for silica

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

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

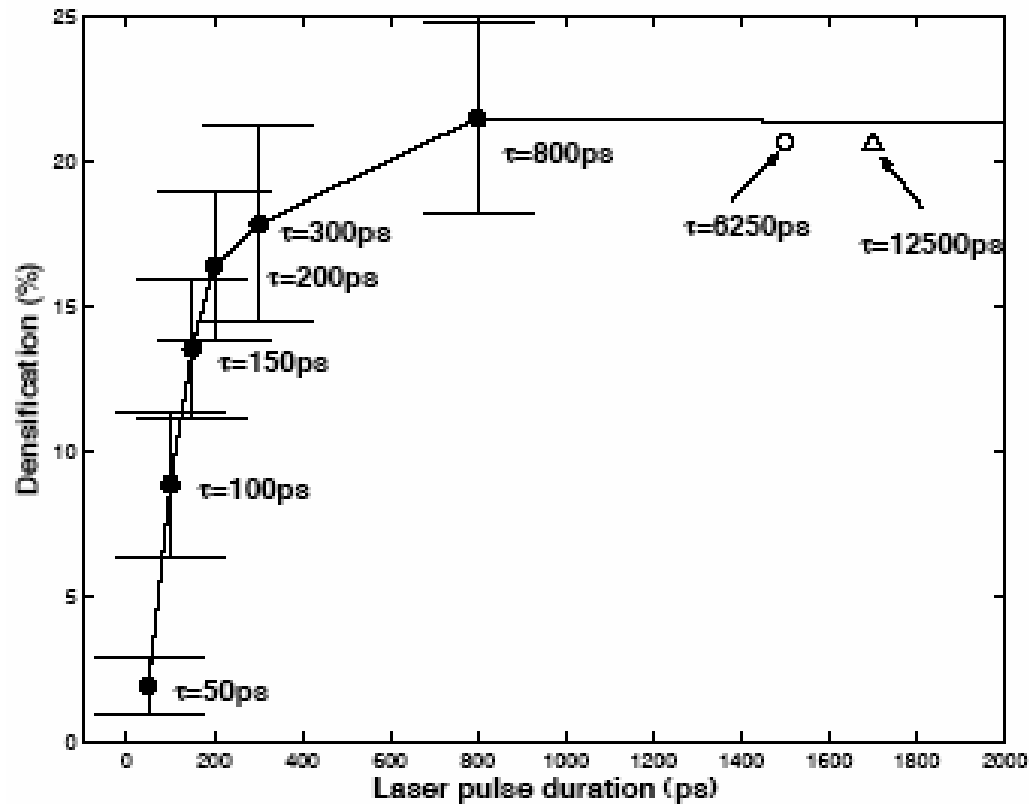


MD LASER IRRADIATION: Effect of pulse duration & absorbed fluence @ $T = 300\text{ K}$, $p = 0\text{ GPa}$



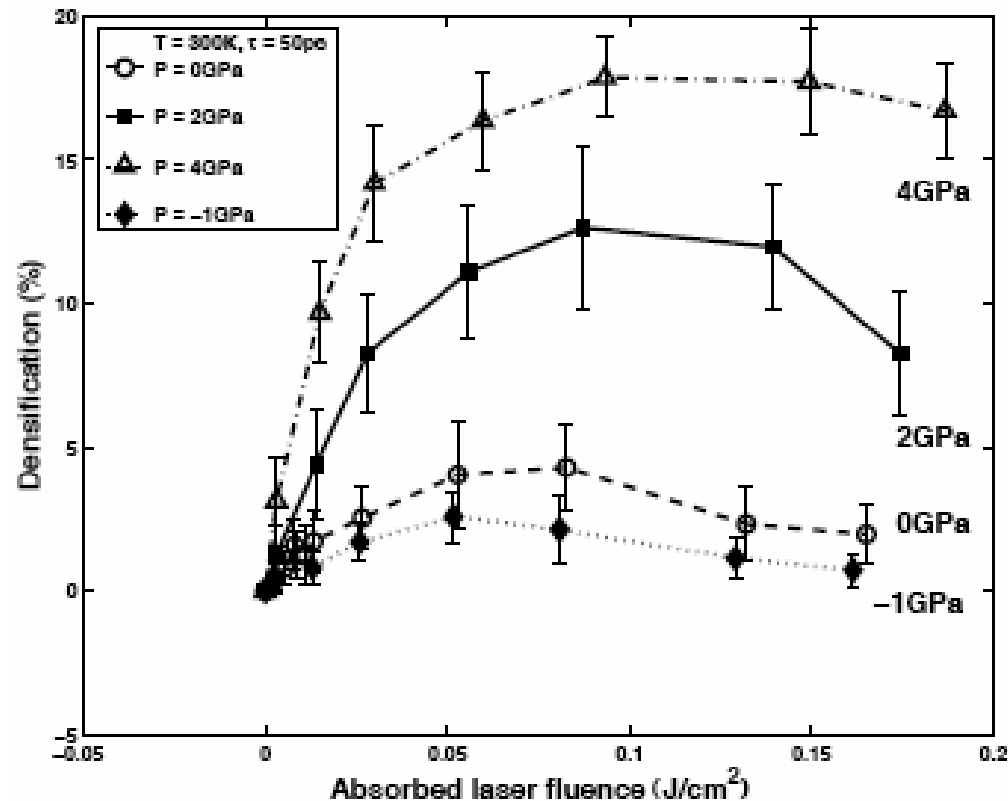
MD LASER IRRADIATION: Effect of pulse duration @ T = 300 K, p = 0 GPa

Absorbed fluence = 0.165 J/cm²

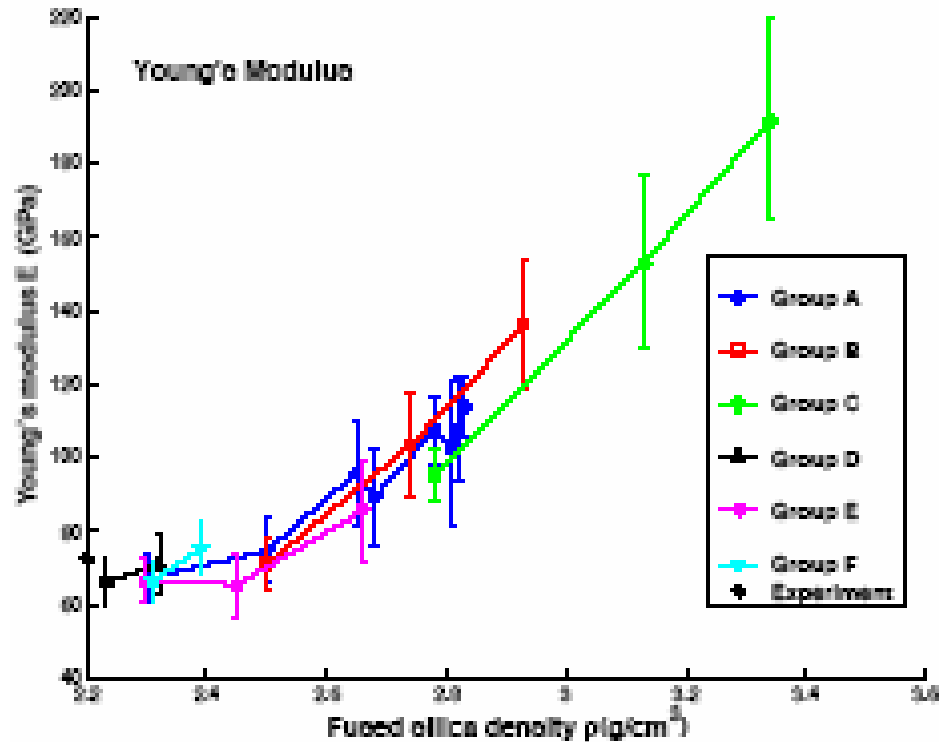


MD LASER IRRADIATION: Effect of pressure @T = 300 K

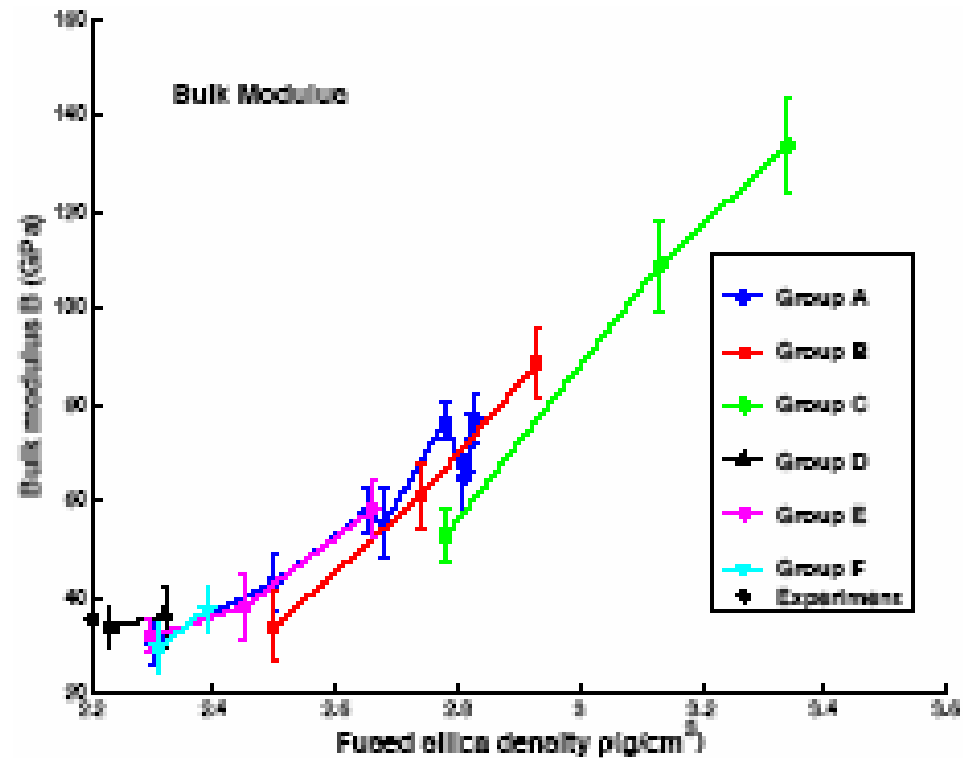
Higher pressure produces higher densification



MD simulations: Effect of radiation on Young's modulus



MD simulations: Effect of radiation on bulk modulus B



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

