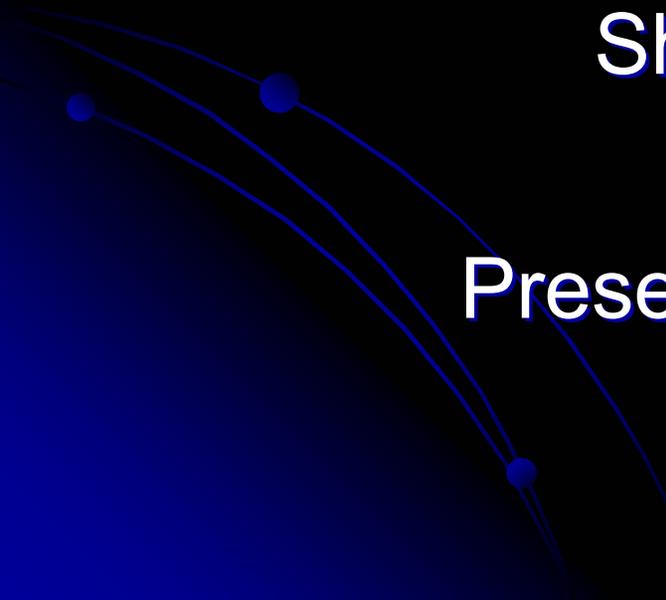


Strength and Elasticity of SiO_2 across the Stishovite- CaCl_2 - type Structural Phase Boundary

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1. Introductions

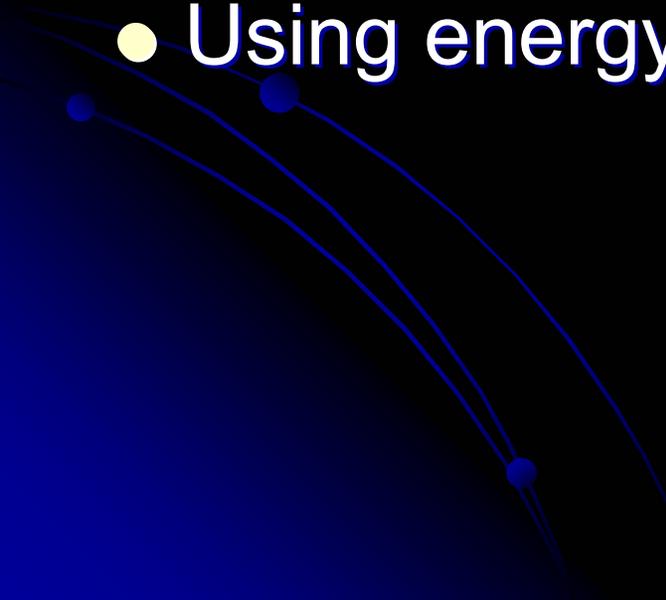
- **Stishovite:** a dense tetragonal polymorph of quartz that is formed under great pressure and is often associated with meteoroid impact. (from Dictionary)
- **Why Stishovite important?**
 1. may explain some seismic structure in the mantle
 2. a prototype for the six-coordinated silicates
 3. transformation: stishovite \rightarrow orthorhombic CaCl_2 structure at ~ 50 GPa

- Elastic properties is important for the understanding of phase transformation.

However, direct experimental measurements of the elastic properties, strength and plastic deformation behavior of stishovite at high pressure is very limited.

- This Paper: use lattice strain meas. under nonhydrostatic compression in a diamond anvil cell to examine dense SiO_2 over a broad pressure range.

2. Experiment

- Pure stishovite powder
 - Au foil: pressure marker and reference for the x-ray position
 - Diamond anvil cell: compress the sample
 - Using energy dispersive x-ray diffraction
- 

3. Data analysis

- Using lattice strain theory to analyze data
- Def. of differential stress $t = \sigma_3 - \sigma_1$
 - σ_3 : stress along the diamond cell axis
 - σ_1 : the radial stress
- The supported t is a lower bound to the yield strength

$$d_m(hkl) = d_p(hkl)[1 + (1 - 3 \cos^2 \psi)Q(hkl)], \quad (1)$$

$$Q(hkl) = (t/3)\{\alpha[2G_R^X(hkl)]^{-1} + (1 - \alpha)(2G_V)^{-1}\}. \quad (2)$$

- $d_m(hkl)$: measured interplanar spacing for plane (hkl) (?)
- $d_p(hkl)$: d spacing resulting from the hydrostatic component of stress
- Ψ : the angle between the diffracting plane normal and the loading direction
- $G_R^X(hkl)$: x-ray shear modulus under Reuss (isostress) condition
- $G_V(hkl)$: x-ray shear modulus under Voigt (isostrain) condition
- α : 0 – 1, weighting factor

- $d_m(hkl) = d_p(hkl)$ when $\Psi = 54.7^\circ$
- t can be estimated from the shear modulus G and the average $Q(hkl)$ value from all measured reflections:

**Peaks shift to lower
Energies as Ψ
increases**

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Shieh, S. R., et al. "Strength and elasticity of SiO₂ across the stishovite-CaCl₂-type structural phase boundary." *Physical Review Letters* 89 (2002): 255507.

FIG. 1. Energy dispersive x-ray diffraction spectra at maximum strain ($\psi = 0^\circ$) and minimum strain ($\psi = 90^\circ$).

- Assume that the measured d spacings correspond to volume compression under hydrostatic stress (?)

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Compression curve is strongly sensitive to Orientation Ψ :
 $\Psi \uparrow \rightarrow d \uparrow \rightarrow V/V_0 \uparrow$
(less incompressible)

FIG. 2. Equation of state at $\psi = 0^\circ, 54.7^\circ$ and 90° . Solid symbols are from this study. Open squares are from Ref. [6] and open triangles are from Refs. [1,14]. The solid line is a fit to our data at $\psi = 54.7^\circ$ using the Birch-Murnaghan equation of state. Error bars are smaller than symbols where not shown.

- Elastic properties reflect the bond strength and directionality, but insufficient for complete characterization since shear strength can vary greatly.
- The ratio of shear strength τ to shear modulus G : $\tau / G \rightarrow$ reflects the contribution of both plastic and elastic deformation.
- This study examines t/G : can be obtained from the average slope of d spacing VS $(1 - 3\cos^2\Psi)$ term (why t , not τ ?)

15 – 60 GPa
0.019 – 0.037

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**The ratio for Stishovite is
about half the value for
olivine and ringwoodite
Below 30 GPa**

FIG. 3. Ratio of differential stress to shear modulus as a function of pressure. Solid circles denote data from this study. Open squares are from Ref. [29]. Open diamonds are from Ref. [24]. The upward and downward pointing triangles are calculated from the data of Ref. [9] and Ref. [10], respectively (see text for detail).

Differential stresses supported by stishovite are significantly lower than those of ringwoodite, consistent with measurements on SiO₂ glass

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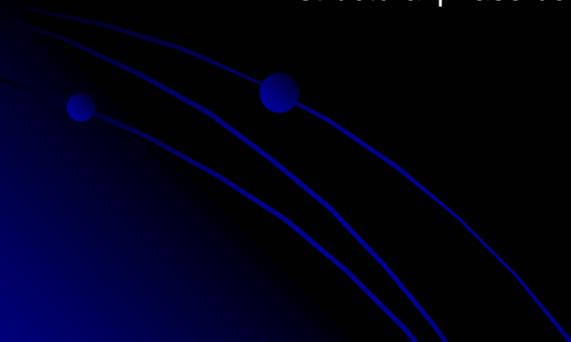


FIG. 4. Differential stress supported by stishovite as a function of pressure. Solid symbols are from this study with a fit to the data shown by the solid line. Open squares and diamonds are from Ref. [29] and Ref. [24], respectively.

- Use lattice strain equations to recover full elastic stiffness tensor at high P.
- Shishovite in tetragonal system has six independent elastic stiffness (C11, C12, C13, C33, C44, C66). Lattice equations are insensitive to C44 and C66, so these two were fixed to theoretical values. → 4 unknowns
- 6 knowns (4 independent lattice reflections, compressibility, c/a ratio)
- Inversion equations:

$$1/K = 2S_{11} + 2S_{12} + 4S_{13} + S_{33}, \quad (4)$$

$$d \ln(c/a)/dP = S_{11} + S_{12} - S_{13} - S_{33}, \quad (5)$$

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FIG. 5. Elastic moduli as a function of pressure from this study (solid circles and lines) and Refs. [8–10]. Dotted lines, Ref. [10]; open triangles and dash-dotted lines, Ref. [8]; open squares and dashed lines, Ref. [9].

4. Conclusions

- The ratio of differential stress to shear modulus t/G is 0.019 – 0.037 at $P = 15-60$ GPa
- The ratio for octahedrally coordinated stishovite is lower by a factor of 2 than observed in four-coordinated silicates.
- The differential stress of stishovite is about 4.5 (1.5) GPa below 40 GPa and to decrease sharply as the stishovite- CaCl_2 -type phase transition boundary is approached.
- Inversion of measured lattice strains provides direct experimental evidence for softening of

$$C_{11} - C_{12}$$