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Superhard Materials Under Pressure: Strength and Elasticity of Stishovite

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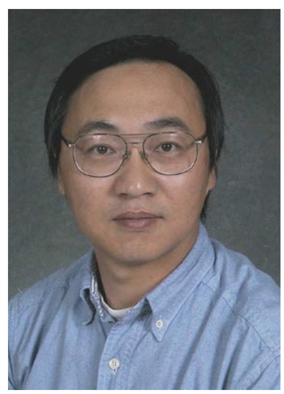
Stishovite, a six-coordinated form of SiO_2 and one of the hardest known oxides, was compressed in a diamond anvil cell to study its elastic and rheological behavior at extreme pressures. Our results show that the yield strength is surprising low at high pressures compared with other silicates. Furthermore, we provide experimental confirmation of the prediction that the transition from stishovite to the $CaCl_2$-type structure near 50 GPa is accompanied by an elastic instability. These results show that application of high pressures can greatly modify expectations of material behavior based on low-pressure considerations.

Stishovite is likely to be an important constituent of the Earth's deep mantle. It is also a prototype for the six-coordinated silicates that are of fundamental importance in geophysics and materials science. The nature of the transformation of stishovite from the rutile structure to the $CaCl_2$-type structure near 50 GPa has been the focus of much recent interest. Stishovite is also among the strongest known oxides, and understanding its elastic and rheological properties is fundamental to the search for new superhard materials. In this study, we use new compression measurement techniques in a diamond anvil cell to examine the elasticity and yield strength of dense SiO_2 over a broad pressure range for the first time.

Stishovite was loaded into a diamond anvil cell and compressed non-hydrostatically. Energy dispersive x-ray diffraction experiments were conducted at beamline X17C at the National Synchrotron Light Source (**Figure 1**). The sample was contained within an x-ray transparent (beryllium) gasket, which enabled us to measure the diffraction pattern at any angle with respect to the loading axis of the cell. The data were analyzed using lattice strain theory, which relates the anisotropy of the measured lattice strains to the yield strength and the elastic stiffness coefficients.

Figure 2 shows the yield strength of stishovite as a function of pressure from our x-ray diffraction data combined with theoretical predictions for the shear modulus. The yield strength was found to be nearly constant at pressures of 15-40 GPa and dropped sharply as the transition pressure was approached. The yield strength then increased rapidly in the $CaCl_2$-type phase. In contrast to its ambient-pressure behavior, our measurements indicate that the yield strength of stishovite is surprisingly low at high pressures especially when compared with other silicates (e.g. ringwoodite).



Authors (Clockwise from left): Sean R. Shieh, Baosheng Li, and Thomas S. Duffy

Our data also allow for inversion to recover a partial elastic stiffness tensor at high pressure. In general, our values of C_{11} and C_{12} (**Figure 3**) lie below theoretical values, but they are qualitatively consistent with theory in that C_{11}-C_{12} is markedly reduced near the transition pressure. This provides direct experimental support for the theoretical prediction of an elastic instability involving C_{11}-C_{12} in stishovite near 50 GPa.

This study of stishovite provides an example of how recent developments in diamond anvil cell technology together with synchrotron x-ray diffraction techniques are yielding new advances in our understanding of fundamental quantities such as elasticity and yield strength of strong materials under extreme pressure conditions.

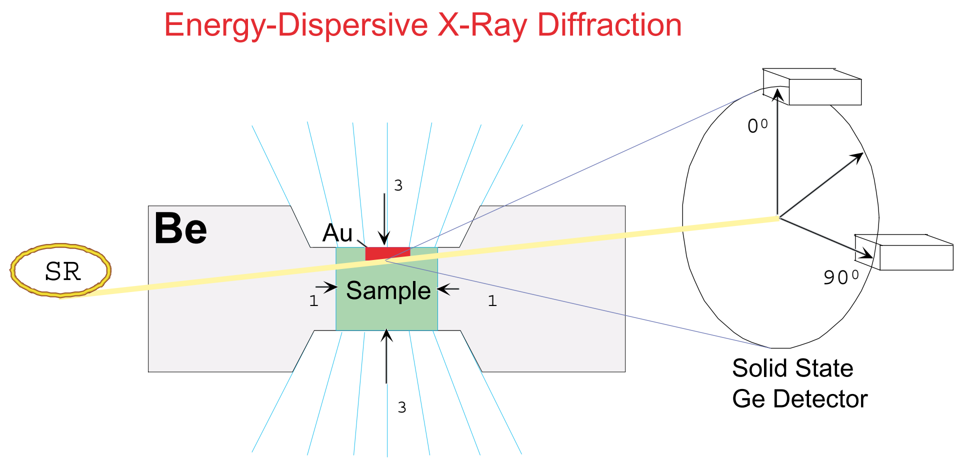


Figure 1. *Sample configuration for radial x-ray diffraction experiments in a diamond anvil cell. The incident x-ray beam was directed through beryllium gasket instead of the conventional diamond window. The diffraction patterns of both sample and pressure standard are recorded by a solid-state Ge detector. The Au foil is used as a pressure marker, and σ_3 and σ_1 represent maximum and minimum stresses. Rotation of the sample allows lattice strains to be recorded at both the minimum and maximum stress directions.*

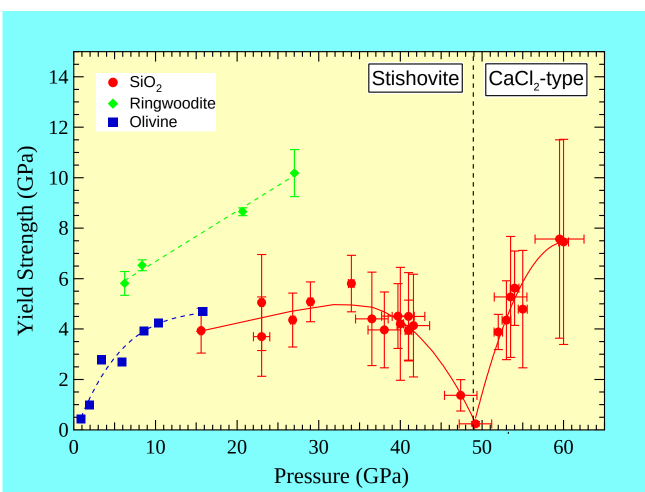


Figure 2. *Yield strength of stishovite at high pressure. Red symbols and line are from this study; Squares and diamonds are olivine (α-Mg_2SiO_4) and ringwoodite (γ-Mg_2SiO_4) data, respectively. Dashed line shows the transition boundary of stishovite to the $CaCl_2$-type.*

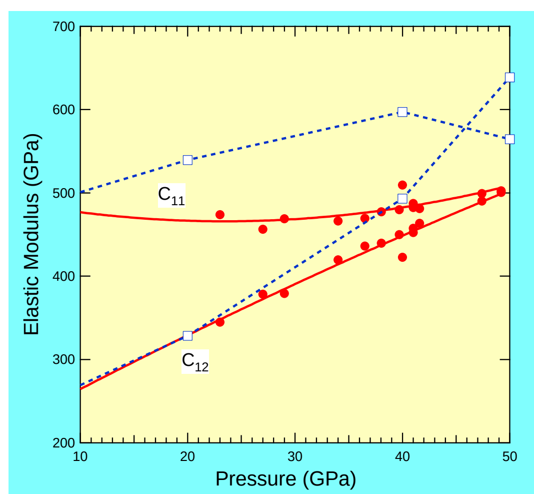


Figure 3. *Selected elastic moduli of stishovite at high pressure. Red symbols and line are from this study; open symbols and dashed lines are from theoretical calculations.*