Polyamorphic Transitions in B_2O_3 glass

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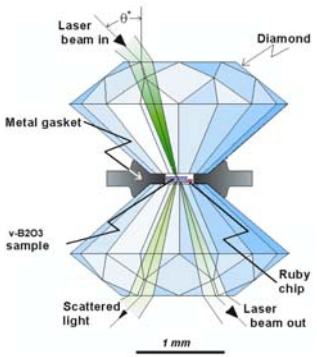
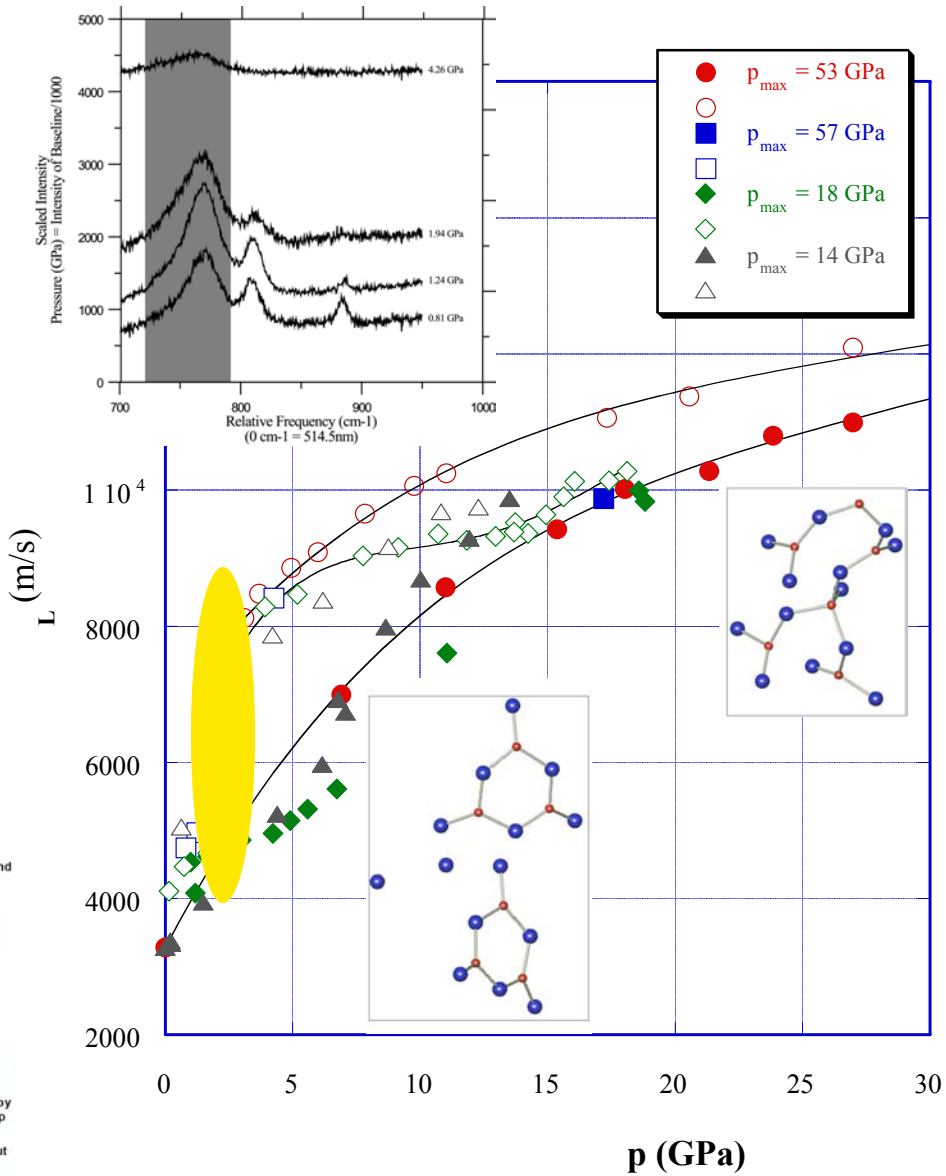
Polyamorphism, i.e., the existence of two distinct non-crystalline states for the same material, has been evidenced for vitreous B_2O_3. The pressure-induced transformation between low-density and high-density B_2O_3 is continuous upon compression and 1st-order upon de-compression, as revealed by the change in sound velocity.

Molecular dynamics simulations showed that a significant fraction of boron transitions from trigonal (BO_3-units) to tetrahedral (BO_4-units) coordination.



High-pressure Brillouin scattering experiments are carried out using a diamond anvil cell. The specimen in enclosed between flattened diamond tips by a metal gasket. The diamonds allow for the application of high pressures and act as windows for the probing radiation.



Thermo-mechanical Anomalies and Permanent Densification in Silica Glass

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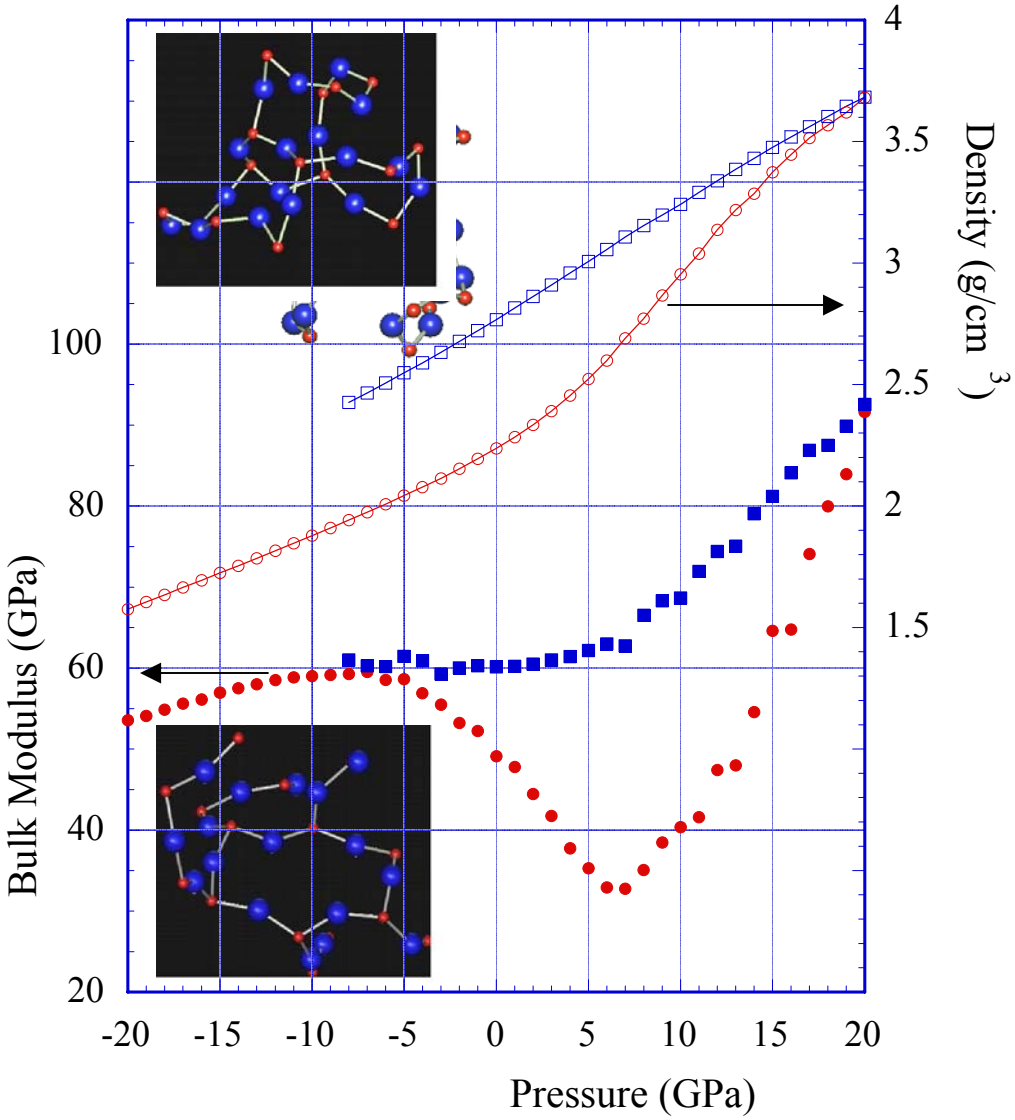
Molecular dynamics simulations of silica glass reveal that the anomalous decrease of the elastic modulus with increasing pressure is due to the abrupt and localized structural transitions, following a mechanism similar to that underlying the α-to-β transformation in cristobalite.

Permanent densification involves the formation of larger rings. The degree of permanent densification in the recovered glass increases with increasing temperature.

Densified glass no longer exhibits anomalous thermo-mechanical behavior.



Polyamorphism, Structural Transitions, and Related Phenomena

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Education:

Four undergraduate (Ranjeet Rao, Surair Bashir, Vashist Vasanthakumar, Peter Gullekson) and two graduate students (Liping Huang and Jason Nicholas) contributed to this work.

Ranjeet is now a graduate student at the University of Illinois and recipient of an NSF Graduate Fellowship. Surair (an African-American female), Vashist, and Peter are undergraduates at Michigan. Peter is still involved in the project.

Jason has graduated with an M.S. degree in May '03, and is now a Ph.D. student at U.C. Berkeley.

Liping received her Ph.D. in May '04. As the 2003 recipient of the Norbert J. Kreidl Award from the ACerS, she was invited to give a featured lecture on her simulation work during the Norbert J. Kreidl Memorial Conference, June 23-26, 2004, in Slovakia.

Outreach:

The PI is co-organizer and participant in the Materials Camp held annually at Michigan. 20 high school science teachers spend a week learning about materials science, with the goal of using this information in their curricula and teach high school students about the role of materials in technology.