Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Mechanical strength and coordination defects in compressed silica glass YUNFENG LIANG, International School for Advanced Studies (SISSA) and INFM-CNR Democritos National Simulation Center, Trieste (Italy), CAETANO R. MIRANDA, SANDRO SCANDOLO, The Abdus Salam International Centre for Theoretical Physics (ICTP) and INFM-CNR Democritos National Simulation Center, Trieste (Italy) — Contrary to ordinary solids, which are normally known to harden by compression, the mechanical strength of compressed SiO_2 glass shows a minimum around 10 GPa. Around this pressure, the compression of silica glass undergoes a change from purely elastic to plastic, leading to the recovery of a densified amorphous polymorph. The compressibility of silica glass is also anomalous, with a maximum at about 2-4 GPa. Despite the large pressure difference between the onset of the two anomalies, microscopic theories have traditionally attempted to explain both anomalies with the pressure induced appearance of coordination defects. Such models are seriously questioned however by the lack of evidence for coordination defects below 10 GPa, in Raman and NMR experiments. Here we show, using an improved interatomic potential for SiO_2, that a correct description of the pressure-induced appearance of five-fold coordination defects in silica glass is crucial to address the above phenomenology and to obtain a theoretical model consistent with experiments.

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Date submitted: 13 Dec 2005 Electronic form version 1.4