

Amorphous Silica obtained from the Zeolite Chabazite due to Structural Collapse under Mild Pressure-Temperature Conditions

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Abstract

The siliceous zeolite chabazite, which has a very large void volume for a crystalline silica polymorph, was found by *in situ* synchrotron, x-ray diffraction in diamond anvils cells to collapse and become amorphous under mild, pressure-temperature conditions in the range of 0.5-1 GPa and 320-454 K. This procedure was scaled up under technologically-relevant conditions of around 0.7 GPa and 473 K in a standard pellet pressing die equipped with a band heater. The materials obtained are distinct from silica glass with first sharp diffraction peaks at close to $1.60\text{-}1.63\text{ \AA}^{-1}$, shorter intertetrahedral distances, and different infrared spectra. The mechanism for this collapse is dominated by the closure of the 8-membered rings of SiO_4 tetrahedra in the large chabazite cages in the structure resulting in a close to 40 % decrease in volume almost entirely due to the reduction of the c lattice parameter of rhombohedral chabazite. These results open the way to obtain novel amorphous forms of silica with characteristic medium-range order under mild *P-T* conditions, which could be expected to have distinct optical and mechanical properties with respect to silica glass.

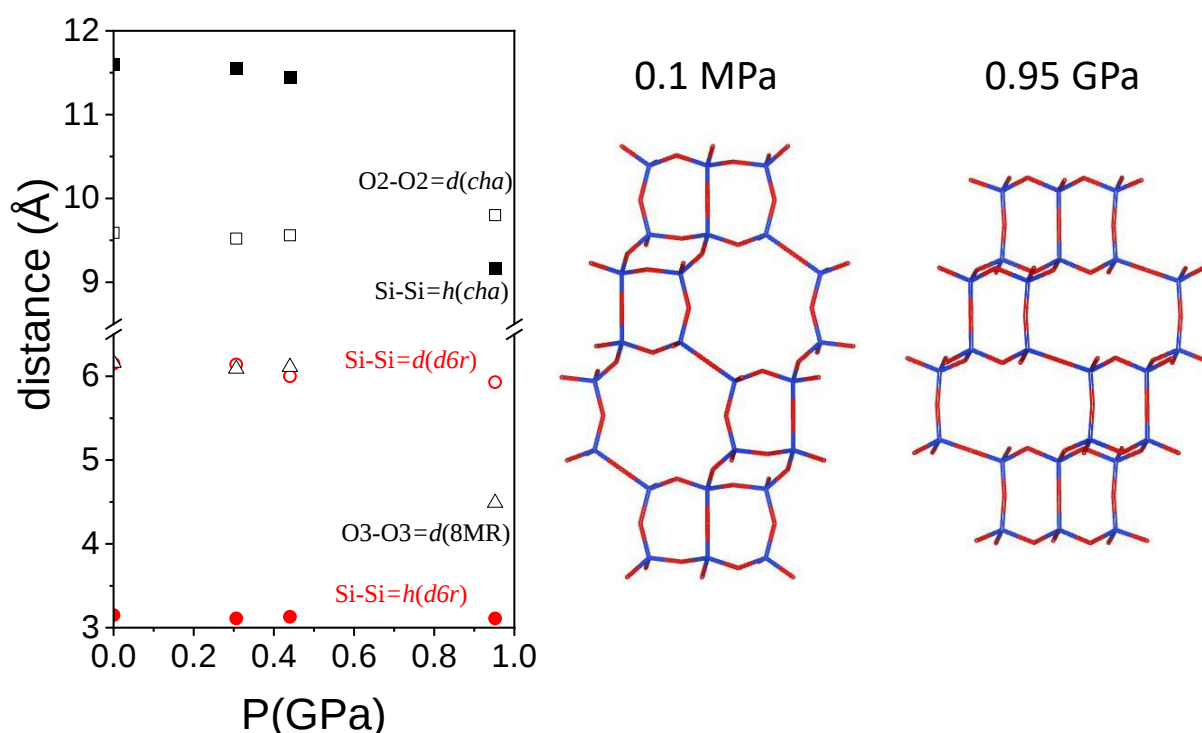


Figure 1 Selected interatomic distances in CHA as a function of pressure (left). Details of the crystal structure (right) of CHA at 0.1 MPa and 0.95 GPa. Bonds are represented in blue (Si-extremity) and red (O-extremity).