

## Supplementary Materials for **Picosecond amorphization of SiO<sub>2</sub> stishovite under tension**

Masaaki Misawa, Emina Ryuo, Kimiko Yoshida, Rajiv K. Kalia, Aiichiro Nakano, Norimasa Nishiyama, Fuyuki Shimojo, Priya Vashishta, Fumihiro Wakai

Published 12 May 2017, *Sci. Adv.* **3**, e1602339 (2017)  
DOI: 10.1126/sciadv.1602339

### The PDF file includes:

- Legends for movies S1 and S2
- fig. S1. Si-Si and O-O pair distributions at various densities.
- fig. S2. Change of coordination numbers and bond-angle distributions during the stishovite-to-amorphous transformation.
- fig. S3. Atomic displacements during the stishovite-to-amorphous transformation.

### Other Supplementary Material for this manuscript includes the following: (available at [advances.sciencemag.org/cgi/content/full/3/5/e1602339/DC1](http://advances.sciencemag.org/cgi/content/full/3/5/e1602339/DC1))

- movie S1 (.mov format). Rapid amorphization of stishovite upon volume expansion at a critical tension of  $-30$  GPa.
- movie S2 (.mov format). Change of atomic configurations along the reaction pathway from the stishovite to amorphous phases at  $\rho = 3.4$  g/cm<sup>3</sup>.

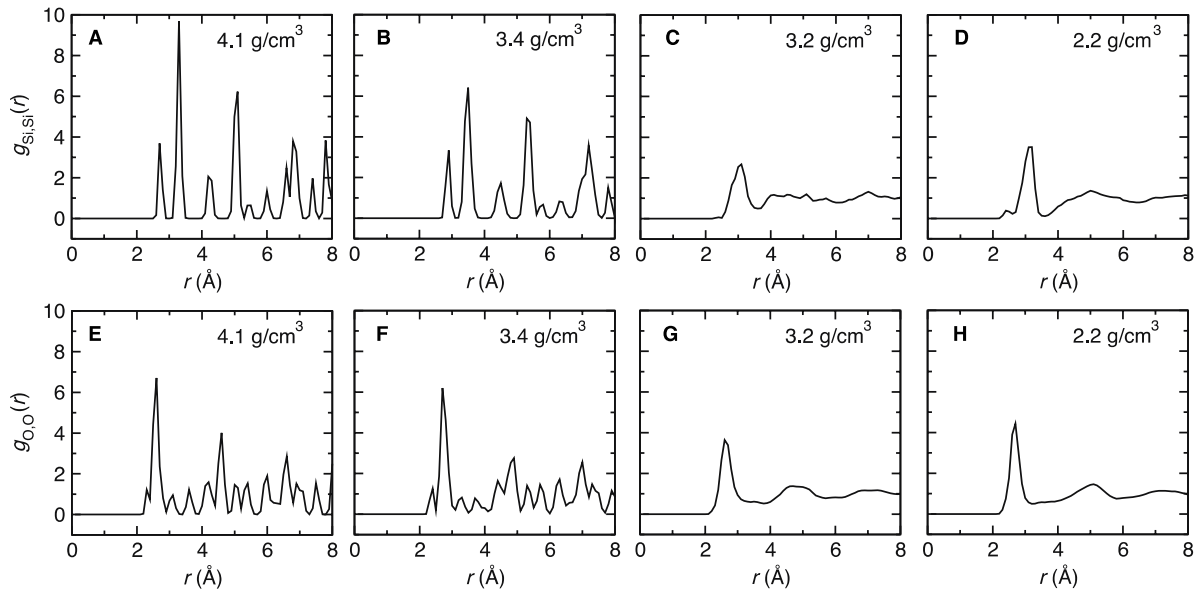
## Supplementary Materials

### Video captions

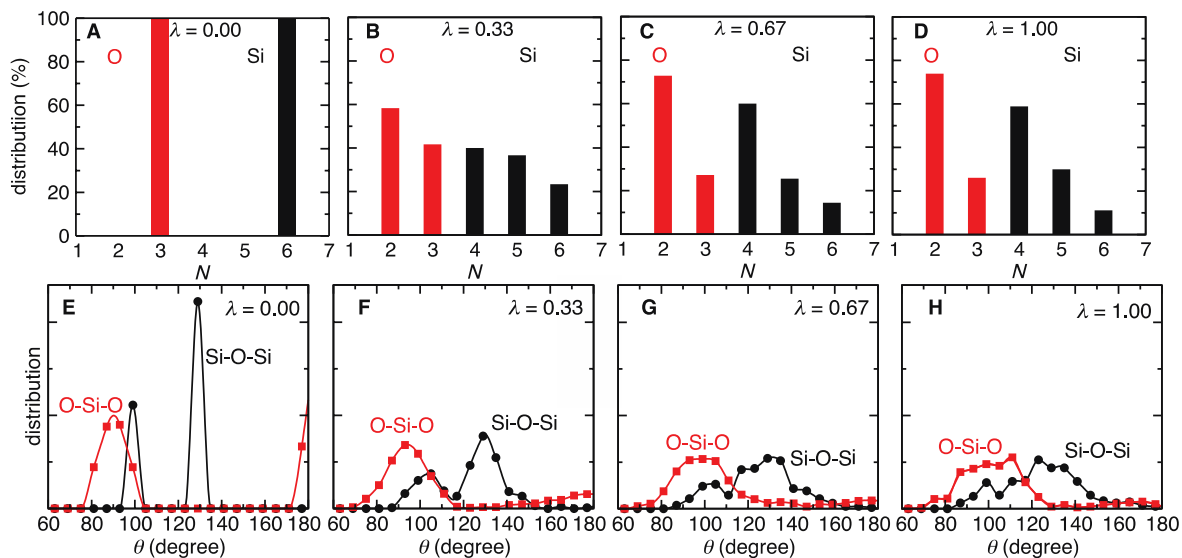
**movie S1. Rapid amorphization of stishovite upon volume expansion at a critical tension of  $-30$  GPa.** The yellow and red spheres indicate Si and O atoms, respectively.

**movie S2. Change of atomic configurations along the reaction pathway from the stishovite to amorphous phases at  $\rho = 3.4$  g/cm<sup>3</sup>.**

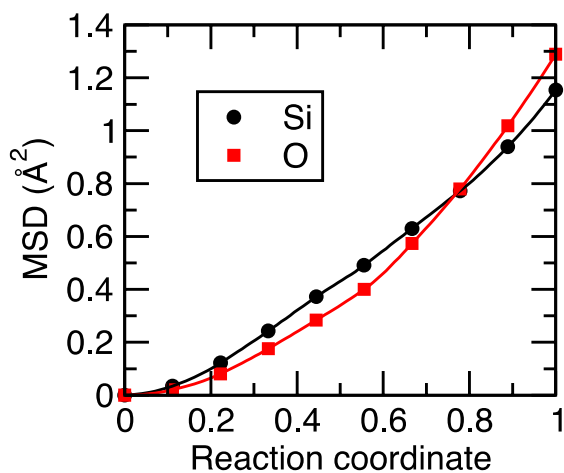
### Supplementary figures



**fig. S1. Si-Si and O-O pair distributions at various densities.** Partial pair-distribution functions  $g_{\alpha\beta}(r)$  for  $\alpha-\beta =$  Si-Si (**A to D**) and O-O (**E to H**) at various mass densities.



**fig. S2. Change of coordination numbers and bond-angle distributions during the stishovite-to-amorphous transformation.** Distributions of the coordination number of Si (black) and O (red) atoms (**A** to **D**) and distributions of the bond angles  $\theta_{\alpha-\beta-\gamma}$  for  $\alpha-\beta-\gamma = \text{Si-O-Si}$  (black) and O-Si-O (red) (**E** to **H**) at reaction coordinate  $\lambda = 0.0, 0.33, 0.67$  and  $1.00$  along the stishovite-to-amorphous transformation at  $\rho = 3.4 \text{ g/cm}^3$ .



**fig. S3. Atomic displacements during the stishovite-to-amorphous transformation.** Black circles and red squares denote the MSDs of Si and O atoms, respectively, along the reaction coordinate during NEB calculation of stishovite-to-amorphous transformation at  $\rho = 3.4 \text{ g/cm}^3$ .