

The details of obtaining the material parameters of amorphous silica are introduced as follows. In this paper, the Morse potential is adopted for silica, i.e.

$$V_{ij}(r_{ij}) = \frac{q_i q_j}{r_{ij}} + D_0 [e^{a(1-\rho_{ij})} - 2e^{a(1-\rho_{ij})/2}] \quad \backslash * \quad \text{MERGEFORMAT}$$

$$\rho_{ij} = r_{ij} / r_0$$

(1)

Where V_{ij} are the potential energy between atom i and atom j ; r_{ij} is the distance between the two atoms; r_0 represents equilibrium distance; q_i and q_j are the charge of the two atoms, respectively. The parameters in Eq. \(* MERGEFORMAT (1) have been given in literature.¹ During MD simulation, the particle-particle particle-mesh (PPPM)² method is employed to compute the coulomb interaction; the cutoff radius and time step are taken as 10Å and 1.0fs, respectively.

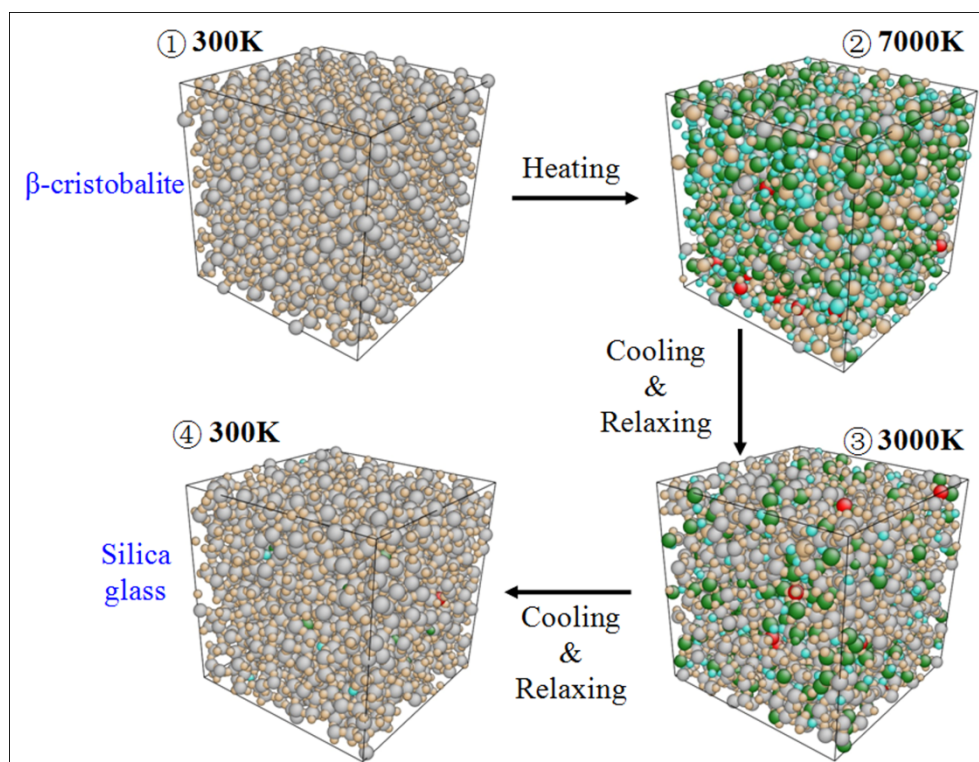


Fig. 1 The preparation of numerical sample of silica glass in MD simulation.

Fig. 1 shows the preparation of silica glass using the melt-quenching method in MD simulation. Firstly, the β -cristobalite structure with 5184 atoms is established in a cubic simulation box with periodic boundary conditions. The β -cristobalite is melted

at 7000K for 200ps in NVT ensemble. A multi-steps quenching scheme is adopted to quench silica liquid to silica glass from 7000K to 300K: the quenching rate is 5K/ps and the system is equilibrated at each 1000K for 50ps. Finally, the amorphous sample is relaxed at 300K for 200ps in NPT ensemble.

The elastic properties of silica glass are obtained similar to the method in the work of Yuan and Huang.³ The numerical sample consisted of 5184×2 atoms is used for uniaxial test with a strain rate of $10^9/s$. The NPT assemble is adopted during uniaxial tension or compression test. In this case, the lateral directions are relaxed to keep zero lateral pressure while the loading direction is elongated or constricted. The simulation results are shown in Fig. 2, including tensile and compressive stress-strain curves. The slope of initial linear segment is calculated to be 72.56GPa, which is considered as the Young's modulus of silica glass. The Poisson's ratio is calculated to be 0.17, which is the ratio of the lateral shrinkage to the longitudinal elongation within the linear segment.

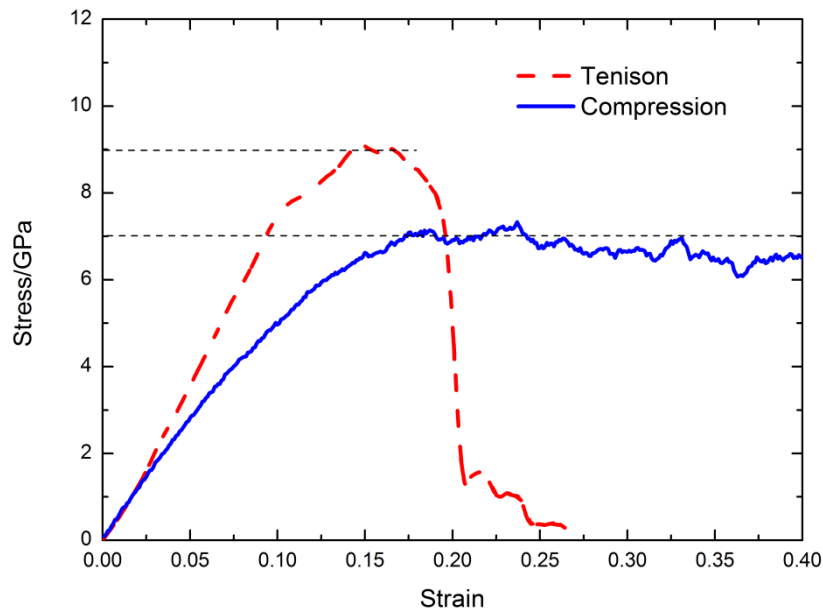


Fig. 2 The uniaxial stress-strain curves of silica glass in MD simulation.

The surface energy of silica glass are obtained as shown in Fig. 3 similar to the method of Frolov and Mishin.⁴ Firstly, a numerical sample is equilibrated under periodic boundary conditions (Fig. 3①). In this case, the potential energy of each

atom (E^{atom}) can be expressed as

$$E^{atom} = E^{bulk} / N_{bulk} \quad \backslash * \text{MERGEFORMAT (2)}$$

Where E^{bulk} and N_{bulk} are the total potential energy and numbers of all atoms in Fig. 3①, respectively. Next, the simulation box is enlarged in one direction and the system is fully equilibrated (Fig. 3②). Two plates are cut out of the bulk, and then moved to be far from each other (Fig. 3③). Finally, the surface energy (γ_s) of silica glass can be computed by

$$\gamma_s = (E^{slab} - N_{slab}E^{atom}) / (4A_s) \quad \backslash * \text{MERGEFORMAT (3)}$$

Where E^{slab} and N_{slab} are the total potential energy and numbers of all atoms in Fig. 3③, respectively. In this paper, the numerical model contains 5184 atoms, and the initial simulation box size is 42.5×42.5×42.5nm. Finally, the surface energy of silica glass is calculated to be 1.14J/m².

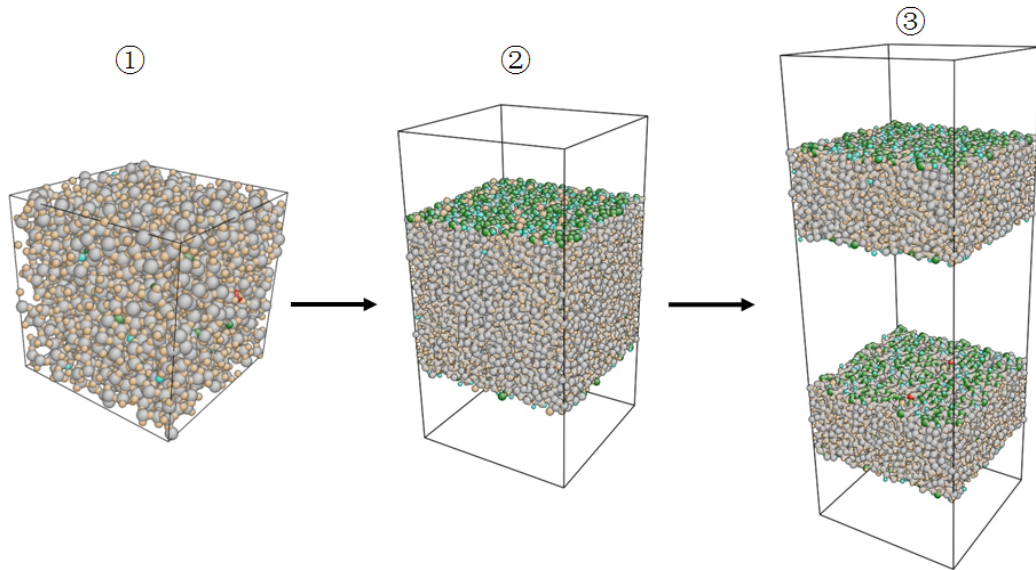


Fig. 3 The procedure of computing the surface energy of silica glass in MD simulation.

Reference

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2. R. W. Hockney and J. W. Eastwood, *Computer simulation using particles*, CRC Press, 1988.
3. F. Yuan and L. Huang, *Journal of Non-Crystalline Solids*, 2012.
4. T. Frolov and Y. Mishin, *Physical Review B*, 2009, **79**, 045430.