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Molecular Dynamics Simulation of Mechanical Properties for α-SiO_2 Crystal

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Abstract

The mechanical properties of the α-SiO_2 crystal are studied by molecular dynamics method with Tersoff potential function. The results show that the α-SiO_2 crystal goes through elastic deformation, plastic deformation and fracture deformation in the process of uniaxial loading at room temperature. The α-SiO_2 is from crystal phase transformation to amorphous phase in plastic deformation. And also by studying the influence of temperature on the tensile mechanical properties of α-SiO_2, it finds that the yield strength and elastic modulus of α-SiO_2 decrease gradually as the temperature increases. Moreover, the higher the temperature, the lower the fracture stress and fracture strain; the α-SiO_2 crystal is easy to be broke under high temperature uniaxial loading. And it also finds that the crack is able to decrease the mechanical properties of α-SiO_2 crystal.

Keywords

Mechanical Properties, Tensile, Molecular Dynamics

1. Introduction

The α-SiO_2 is the stable crystal at normal temperature. The research for α-SiO_2 crystal is mainly focused on the phase transition of amortization under high pressure. For example, Wang *et al.* [1] study the structural transformation of α-SiO_2 crystal under high temperature and high pressure, and point out that α-SiO_2 crystal is able to be synthesized on a small scale coesite under high temperature and high pressure. Palmer *et al.* [2] find the phase transition rule of α-SiO_2 by studying the pressurized phase transition process at room temperature. Zhang *et al.* [3] study the structural transformation of α-SiO_2 crystal at high temperature and high pressure and the experimental conditions of coesite formation through mechanical ball milling. Dubrovinsky *et al.* [4] study the

high-pressure phase transition of α-SiO_2, the results show that it obtains another phase structure of α-SiO_2 similar to the structure of α-PbO_2, and find that the stress between 25 GPa and 35 GPa resulting in an amorphous transformation, which is completely amorphous after unloading stress. However, with the rapid development of computer in recent years, it has become possible to study the mechanical properties, structural transformation and physical characteristics of crystal materials by means of large-scale parallel computation using molecular dynamics simulation [5] [6] [7] [8] [9]. For instance, Pan [10] simulates the high-pressure phase transition of α-SiO_2 with Morse potential using molecular dynamics simulation, and points out that the amorphous phase transition occurs when the stress of crystal is higher than 24.6 GPa, and the calculated results are in agreement with the experimental results. Therefore, computer simulations open up another effective way to study the mechanical properties of crystal, which can provide theoretical support for experimental research.

This paper is focused on investigating the basic mechanical properties of α-SiO_2 using molecular dynamics simulation. The stress-strain curves of α-SiO_2 have been studied with the temperature increasing. And the variation of yield stress, yield strain and elastic modulus is discussed for α-SiO_2 crystal in the process of uniaxial tension. The influence law of temperature on tensile mechanical properties is also discussed to comprehensively evaluate the mechanical properties of α-SiO_2. Meanwhile, it constructs the crack models of α-SiO_2 and analyzes the influence of crack on mechanical properties.

2. Atomistic Model and Simulation Method

Figure 1 shows the crystal structure of α-SiO_2. In silicon dioxide, silicon is located at the center of the tetrahedron, and four oxygen atoms are located at the four top angles of the tetrahedron. And then put the tetrahedron structure of SiO_2 into the body-center cubic and construct a crystal cell of α-SiO_2 as shown in Figure 1(A). Then the crystal structure of α-SiO_2 is established according to the Cartesian coordinates as shown in Figure 1(B). Where, the lattice constant a = 4.978 angstrom, b = 4.978 angstrom, c = 6.948 angstrom, the length of the box is $30a \times 30b \times 30c$, the total number of atoms is 324,000, and periodic boundary conditions are used in x-, y- and z-directions.

In molecular dynamics (MD) simulation, the Tersoff potential function [11] is adopted to describe the interaction between Si and O. the model is equilibrated under NPT ensemble at 300 k, and a Nose-Hoover thermostat is applied to maintain the system temperature. Figure 2 present the energy variation of the model in relaxation process, it can be obtained that the crystal model reaches the equilibrium after 10 ps. Then, the model is performed to uniaxial tensile test in z-direction using MD simulation with the time integration step of 1 fs under NPT ensemble. At the same time, the temperatures of 300 K, 500 K, 700 K and 900 K are selected to simulate the tensile mechanical properties of α-SiO_2 crystals at different temperatures. And the LAMMPS code [12] is applied to simulate the tensile mechanical properties.

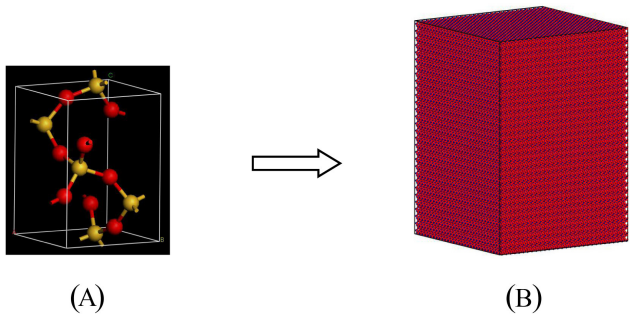

Figure 1. The initial model of α-SiO_2.

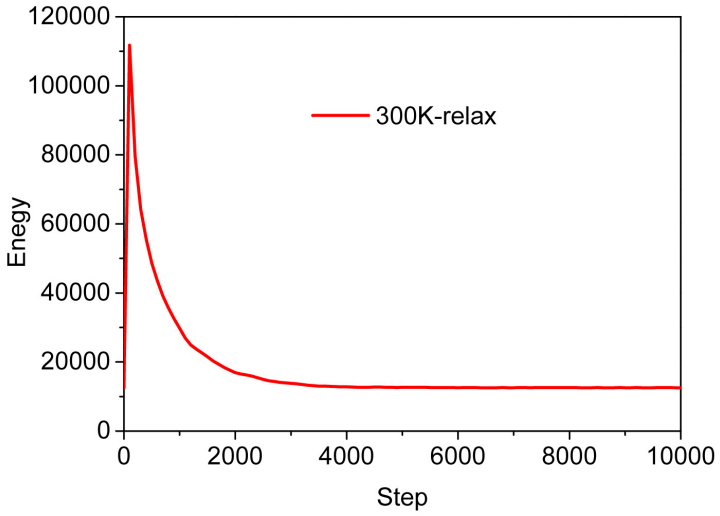

Figure 2. The energy variation of α-SiO_2 in relaxation process.

3. Results and Discussion

3.1. Analysis of Stress-Strain Curve

Figure 3 shows the stress-strain curve of α-SiO_2 under uniaxial tension at room temperature. The yield strain, yield stress, fracture strength and deformation characteristic and so on can be obtained by stress-strain curve, which can reflect the basic mechanical properties of the material. It can be seen from the **Figure 3** that the elastic limit of α-SiO_2 crystal appears when the strain is up to 4.7% (as shown in **Figure 3(A)**), and the stress-strain curve present non-linear relationship. After A, the α-SiO_2 crystal enters the elastic deformation stage. When the strain is up to 32.6%, the stress reaches the first yield point, the yield stress is 22.6 GPa. Then the α-SiO_2 crystal enters the plastic deformation stage, the stress oscillates between point B and point C with the strain increasing, this moment the nanocrystal appears amorphous phase transition. When the stress passes C in **Figure 3**, the crystal structure is completely amorphous, the stress reaches the peak value—fracture strength (36 GPa), the α-SiO_2 crystal enter the stage of fracture. Then the stress falls rapidly to zero as the strain increases and the crystal breaks completely. It can be seen from the **Figure 3** that α-SiO_2 crystal experiences the elastic stage, the plastic stage (amorphous phase transition) and the

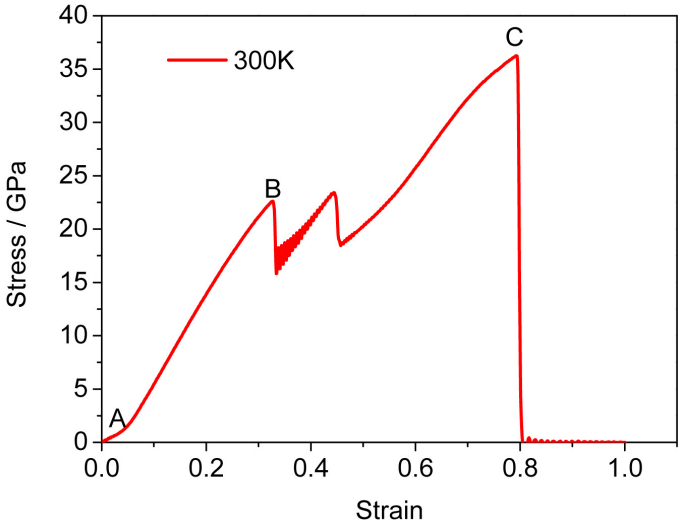

Figure 3. The stress-strain curve of α-SiO_2 in uniaxial tension at room temperature.

fracture stage during the uniaxial tensile process at room temperature, and the elastic modulus reached 69 GPa, so the α-SiO_2 crystal has excellent strength.

3.2. Temperature Effect

In order to discuss the influence of temperature on the tensile mechanical properties of the α-SiO_2 crystal, on the basis of room temperature, the temperatures of 500 K, 700 K and 900 K are selected, and then the mechanical properties of α-SiO_2 crystals are simulated at different temperatures. **Figure 4** shows the variation of the stress-strain curves of the α-SiO_2 crystal at different temperatures. The simulation results show that the yield stress and yield strain decrease with the increasing of temperature. It indicated that the higher the temperature is, the shorter the elastic deformation stage of α-SiO_2 crystal is, and the loading strain of achieving yield strength is smaller. Meanwhile, **Table 1** shows the mechanical parameters of α-SiO_2 under uniaxial tensile at different temperatures, the results present that the elastic modulus decreases gradually with the increasing of temperature. From the data of the calculated elastic model in **Table 1**, the elastic modulus of α-SiO_2 crystal is reduced by 2.3 GPa when the temperature increase from 300 K to 500 K. As the temperature rise from 500 K to 700 K, the elastic modulus of α-SiO_2 crystal is reduced by 1.34 GPa. The elastic modulus decreases by 1.26 GPa as the modulus increases from 700 K to 900 K. It can be concluded that although the elastic modulus of α-SiO_2 crystal decreases as a result of high temperature, but there is no large range of decrease. Therefore, the high temperature only slightly reduces the strength of the α-SiO_2 crystal and does not have much influence on the overall strength.

However, the temperature has a great influence on the fracture strength of the α-SiO_2 crystal. **Figure 5** shows the variation curves of fracture stress and fracture strain at different temperatures. As can be seen from the **Figure 5**, the fracture stress decreases from 36 GPa to 29 GPa with the increasing of temperature,

Table 1. Mechanical parameters of uniaxial tensile of α-SiO_2 at different temperatures.

α-SiO_2	ε_{yield} (GPa)	σ_{yield} (GPa)	E (GPa)
300 K	0.326	22.6	69.32
500 K	0.287	19.24	67.03
700 K	0.274	18.00	65.69
900 K	0.223	14.37	64.43

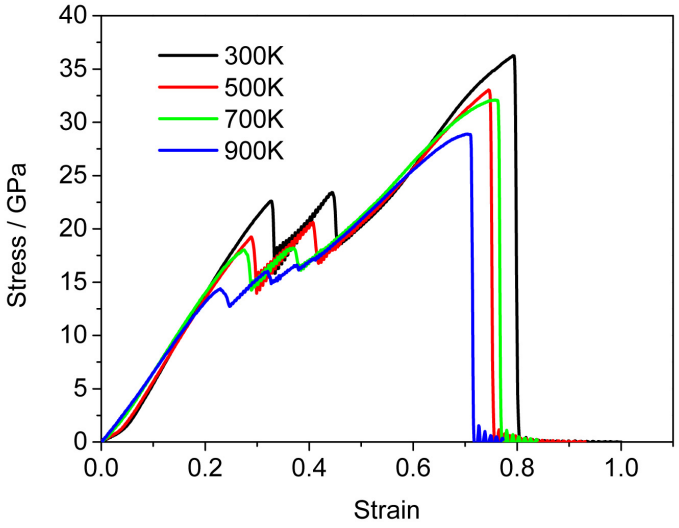

Figure 4. The tensile stress-strain curve of α-SiO_2 at different temperatures.

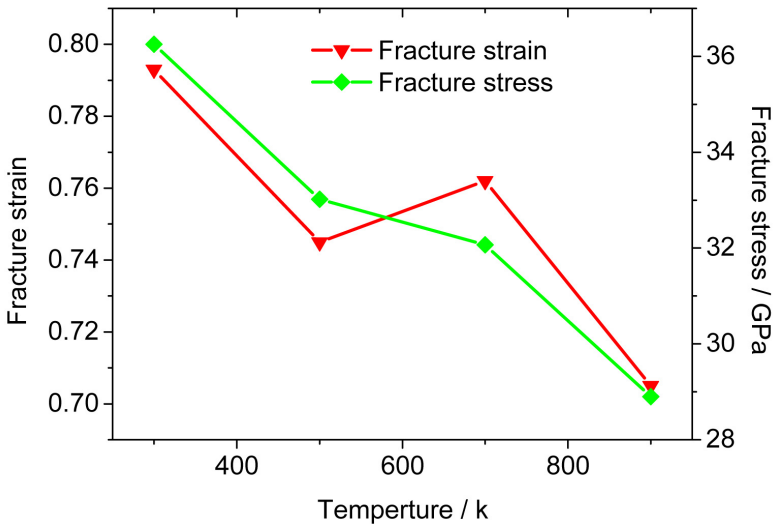

Figure 5. The fracture stress and fracture strain for α-SiO_2 at different temperatures.

which shows a straight downward trend. Although the fracture strain rebound in the process of decreasing with the increasing of temperature, the overall state is also in decline. Therefore, it can be concluded that the higher the temperature is, the lower the fracture stress and fracture strain are, and it is the more easily fracture for α-SiO_2 crystal under high temperature uniaxial loading.

3.3. The Mechanical Properties of Crack Propagation in α-SiO_2 Crystal

In order to discuss the influence of crack on mechanical properties of α-SiO_2 crystal, we construct a crack model by deleting some atoms in α-SiO_2 crystal as shown in Figure 6, and the initial crack length is 2.98 nm. This crack model is then uniaxial stretched for studying the effect of crack on mechanical properties. Figure 7 shows the stress-strain curve of α-SiO_2 crack model at different temperatures. The results present that the yield stress and yield strain decrease with the temperature increasing as shown in Figure 7, the reason is that the crack propagation rate increase with the temperature increasing so that the internal structure is seriously damage at high temperature. Compared to the perfect crystal of α-SiO_2, as the temperature increase from 300 K to 700 K, the crack leads to decreasing of yield stress and yield strain. But the crack model has relatively larger yield stress and yield strain at 900 K, which indicate that the high temperature cause the structure softening so that the crack appear collapse and inhibit the crack rapid propagation.

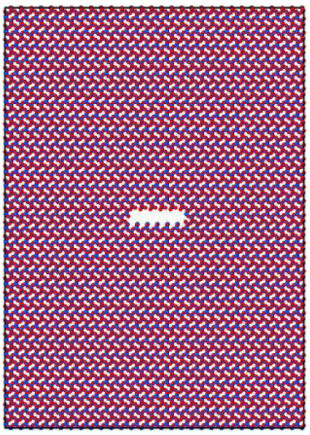

Figure 6. The crack model of α-SiO_2.

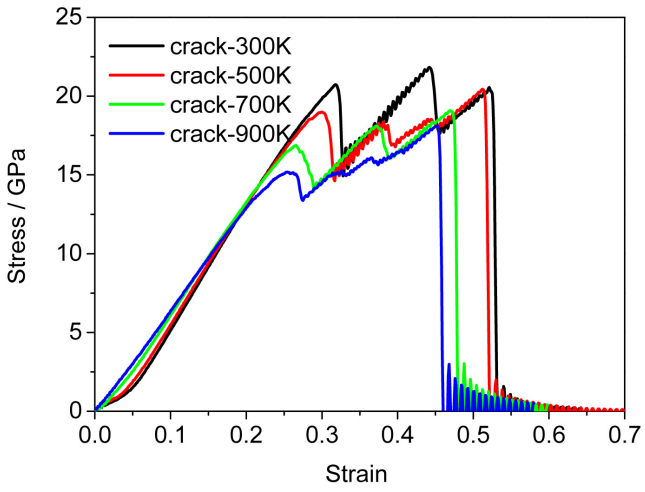

Figure 7. The tensile stress-strain curve of α-SiO_2 crack model at different temperatures.

Table 2. Mechanical parameters of crack model of α-SiO_2 at different temperatures.

α-SiO_2	ε_{yield} (GPa)	σ_{yield} (GPa)	E (GPa)
300 K	0.31	20.7	66.77
500 K	0.30	18.9	62.33
700 K	0.26	16.8	64.61
900 K	0.26	15.1	58.07

And the elastic modulus is obtained by fitting the stress-strain curve of the α-SiO_2 crack model. The calculated values show in Table 2, which present that the elastic modulus of α-SiO_2 crack model vary from 66 GPa to 58 GPa as the temperature arising. Compared to the perfect crystal of α-SiO_2, the elastic modulus of crack model is decreasing at each temperature. So the crack causes the mechanical properties to drop.

4. Conclusion

The tensile mechanical properties of α-SiO_2 crystal are simulated by means of molecular dynamics and with Tersoff potential function. The results show that the α-SiO_2 crystal goes through elastic deformation, plastic deformation and fracture deformation in the process of uniaxial loading at room temperature, and the yield strength is 22.6 GPa, the fracture strength is 36 GPa. The α-SiO_2 is from crystal phase transformation to amorphous phase transition in plastic deformation. And also by studying the influence of temperature on the tensile mechanical properties of α-SiO_2, it finds that the yield strength and elastic modulus of α-SiO_2 decrease gradually as the temperature increases. Moreover, the higher the temperature, the lower the fracture stress and fracture strain; the α-SiO_2 crystal is easy to be broke under high temperature uniaxial loading. The yield stress and yield strain decrease with the temperature increases. For the crack model of α-SiO_2, the yield stress and yield strain decrease with the temperature increases comparing to the perfect crystal of α-SiO_2, and the crack causes the mechanical properties to drop.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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